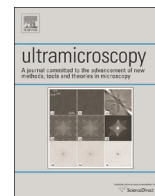




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Extracting features buried within high density atom probe point cloud data through simplicial homology

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ARTICLE INFO

Article history:

Received 1 September 2014

Received in revised form

13 March 2015

Accepted 12 April 2015

Keywords:

APT

Point cloud data

Precipitates

Homology

Topology

AlMgSc

Imaging

ABSTRACT

Feature extraction from Atom Probe Tomography (APT) data is usually performed by repeatedly delineating iso-concentration surfaces of a chemical component of the sample material at different values of concentration threshold, until the user visually determines a satisfactory result in line with prior knowledge. However, this approach allows for important features, buried within the sample, to be visually obscured by the high density and volume ($\sim 10^7$ atoms) of APT data. This work provides a data driven methodology to objectively determine the appropriate concentration threshold for classifying different phases, such as precipitates, by mapping the topology of the APT data set using a concept from algebraic topology termed persistent simplicial homology. A case study of Sc precipitates in an Al–Mg–Sc alloy is presented demonstrating the power of this technique to capture features, such as precise demarcation of Sc clusters and Al segregation at the cluster boundaries, not easily available by routine visual adjustment.

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1. Introduction

Atom Probe Tomography (APT) presents [1–5] enormous potential in probing the sub-nanometer character of materials. However, recovering this information from data generated at such high spatial resolution naturally presents the concomitant challenge of interpreting very high volume and high density data [6,7]. Even small data collections involve $\sim 10^7$ atoms and the standard procedure of visualizing this data set to isolate features can allow important ones, such as precipitates, to be easily lost within the high volume of data. Feature extraction typically requires drawing iso-concentration surfaces [8,9] at a particular concentration threshold, then visually exploring the data space to probe for various features, and repeating the procedure over an entire range of concentration threshold values. Following up on our earlier work in rendering such high volume APT data to aid in feature extraction [10–12] we now provide an alternate data driven approach of objectively classifying different phases such as precipitates by mapping the topology of the APT data set using concepts from algebraic topology, namely, simplicial homology [13–15].

Topology is inherently a classification system that deals with qualitative geometric information. This includes the study of what the connected components of a space are and their connectivity

information in different dimensions of space [16]. Metric properties such as the position of a point, the distance between points, or the curvature of a surface, are irrelevant to topology. Thus, a circle and a square have the same topology although they are geometrically different. Such topological invariants can be represented by simplicial complexes, which are combinatorial objects that can represent spaces and separate the topology of a space from its geometry [14]. Examples of simplices include a point (0-dimensional simplex), a line segment (1-dimensional simplex), a triangle (2-dimensional simplex) and a tetrahedron (3-dimensional simplex).

Simplicial homology is a process that provides information about the simplicial complex by the number of cycles (a type of hole) it contains. One of its informational outcomes are Betti numbers which record the topological invariants of an object, invariants such as the number of connected components, holes, tunnels, or cavities [17]. While a structure can have infinite shapes, many of which cannot be quantified, it can have only limited topological features depending on its dimension. For example, in three dimensions (3D), a structure can be simply connected, or it can be connected such that a tunnel passes through it, or it can be connected to itself such that it encloses a cavity, or it can remain unconnected. Thus, we can characterize the topology of a structure by counting the number of simply connected components, number of tunnels and number of cavities denoted by Betti numbers β_0 , β_1 and β_2 .

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2. Methods

When dealing with point cloud data representing physical structures, such as the APT data, the number and type of topological invariants clearly depends on the degree of connectivity between the various points, established through some metric such as distance. The determination of which points to connect can be addressed by defining a sphere of radius ' ε ' around each point and connecting it to all those other points that lie within this sphere. Again there could be a measure of arbitrariness in determining the appropriate value of ε . A small change in ε for randomly distributed points can quickly change the underlying topology due to statistical noise, thus changing the Betti numbers of the structure. The challenge is to determine the appropriate value of ε that corresponds to a meaningful feature. A powerful technique to overcome this problem is persistent homology [18], so termed because it is based on the idea that betti numbers relating to random distribution of data points and noise cannot persist as we vary ε . The value of ε is gradually increased from 0 and the numbers of different topological components that appear and disappear are tracked for changing ε . This process is called filtration. Only those topological invariants that represent true features in the underlying data will remain unaffected by small changes in ε .

An example of the evolution of Betti numbers with changing ε is shown with 2-D data in Fig. 1. The data points are obtained by sampling 5 points each, at regular intervals, from 3 parallel lines. At $\varepsilon=0$, there are 15 vertices or 0-simplices forming 15 independent components with $\beta_0 = 15$. As the distance threshold for connectivity to adjacent points is increased the vertices connect to their first nearest neighbors resulting in 3 connected components, representing the 3 parallel lines or $\beta_0=3$. As ε is increased further, each point now connects to its second nearest neighbor thus forming 8 squares, each square representing a hole. The whole structure is a single connected component, thus $\beta_0=1$ and $\beta_1=8$. Finally for further increase in ε each vertex now connects to its third nearest neighbor forming triangles, thus, closing the 8 holes. Therefore, $\beta_0=1$ and $\beta_1=0$.

The persistence of different topological features can be recorded as barcodes [Fig. 2] grouped according to each Betti

number. The horizontal axis represents the parameter ε or the range of connectivity around points in the point cloud, while the vertical axis captures the number of topological components present in the point cloud at each interval of ε for β_0 [Fig. 2(a)] and β_1 [Fig. 2(b)]. Initially there are 15 vertices or independent components with $\beta_0=15$ at $\varepsilon=0$. As the distance threshold is increased the vertices connect to their first nearest neighbors forming 3 parallel lines at $\varepsilon=0.5$ resulting in the 15 bars on the barcode plot collapsing into 3 or $\beta_0=3$. If the 3 lines were sufficiently far apart, then the value of $\beta_0=3$ would have persisted for a long duration. However, since the separation between adjacent points is comparable to the separation between points on each line, at $\varepsilon=1$ the points on different lines are interconnected and the whole structure is a single connected component, thus, $\beta_0=1$ thereafter for $\varepsilon \rightarrow \infty$. It should be noted that eventually for $\varepsilon \rightarrow \infty$, the resultant structure will always have $\beta_0=1$ since every vertex will eventually connect to every other one. There has to be some knowledge of the appropriate range for ε , such as the interatomic distance when dealing with raw atom probe data, or voxel length if the data has been voxelized. For β_1 , at $\varepsilon=1$ there are 8 squares, each square representing a hole. Thus, $\beta_1=8$. However, as soon as each vertex connected to its third nearest neighbor, forming triangles, the holes are closed again leading to $\beta_1=0$. The persistence of features is a measure of whether these features are actually present in the data or if they are artifacts appearing at certain intervals. The 8 holes on the β_1 appear for a very short duration and immediately close up.

For the 3D APT data, the sheer number of data points can potentially make the Betti number computation intractable. To overcome this we employ the witness complex [19] construction, which allows us to build a simplicial complex using landmark points sampled from a point cloud data set, carefully chosen to represent the original data. This is demonstrated in Fig. 3 for points sampled from a sphere. The original sampling [Fig. 3(a)] contains about 2000 points and by downsampling [Fig. 3(b)] we can choose about 200 points, which are appropriately spaced.

The points are chosen to be random or evenly spaced. The advantage of even spacing is that it minimizes the probability of statistical noise while on the other hand it necessarily includes

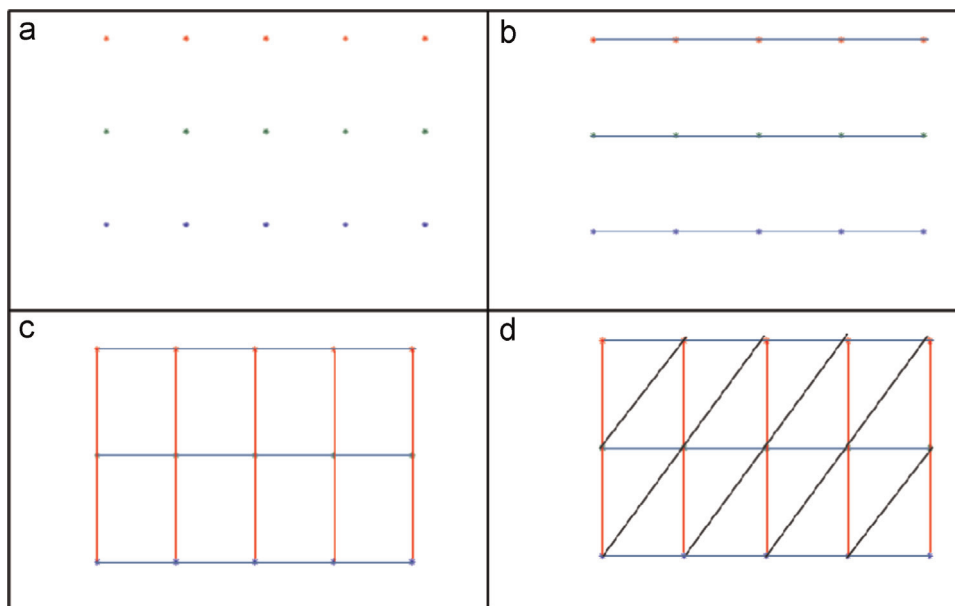


Fig. 1. Persistence in a 2-D point set sampled from a rectangular grid. (a) 15 vertices or 0-simplices forming 15 independent components with $\beta_0 = 15$. (b) As the distance threshold is increased the vertices connect to their first nearest neighbors resulting in 3 connected components (3 parallel lines) or $\beta_0=3$. (c) Each point now connects to its second nearest neighbor thus forming 8 squares, each square representing a hole. The whole structure is a single connected component, thus $\beta_0=1$ and $\beta_1=8$. (d) Each vertex is now connected to its third nearest neighbor forming triangles, thus, closing the 8 holes. Therefore, $\beta_0=1$ and $\beta_1=0$.

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