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Towards an accurate volume reconstruction in atom probe tomography

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ABSTRACT

An alternative concept for the reconstruction of atom probe data is outlined. It is based on the calculation of realistic trajectories of the evaporated ions in a recursive refinement process. To this end, the electrostatic problem is solved on a Delaunay tessellation. To enable the trajectory calculation, the order of reconstruction is inverted with respect to previous reconstruction schemes: the last atom detected is reconstructed first. In this way, the emitter shape, which controls the trajectory, can be defined throughout the duration of the reconstruction. A proof of concept is presented for 3D model tips, containing spherical precipitates or embedded layers of strongly contrasting evaporation thresholds. While the traditional method following Bas et al. generates serious distortions in these cases, a reconstruction with the proposed electrostatically informed approach improves the geometry of layers and particles significantly.

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1. Introduction

Atom Probe Tomography (APT) provides microscopic 3D chemical information in single-atom sensitivity. The analysis is enabled by the field evaporation of individual atoms, which is induced by pronounced electric fields in the order of several tens of V/nm. The required high fields are achieved by means of needle-shaped samples that exhibit a very small apex curvature radius in the range of a few tens of nanometres. With the onset of field evaporation, ionized atoms are emitted from the apex and accelerated towards a position-sensitive 2D detector which records the hit position and the time-of-flight (TOF). While chemical information about the detected events is directly derived from the obtained TOF data, the position data must to be numerically processed. The applied procedure represents the decisive core of the APT method. It leads to the generation of the so-called volume reconstruction: a map of the 3D spatial distribution of the atoms inside the sampled volume with best possible accuracy.

APT instruments do not require a complex ion optics. Instead, the needle-shaped specimen itself acts as the “lens” which controls the image projection and thus the magnification and the imaging quality [1–3]. For this reason, APT is not affected by common lens aberrations, but the ion trajectories may be strongly affected by an unsuitable or at least unknown shape of the tip. If the studied sample material evaporates with constant probability, the physics of field desorption naturally leads to the evolution of a steady, self-similar hemispherical apex shape. In principal, this shape allows the calculation the original launch positions of the ions at the sample surface from the measured detector hit positions. However already in this apparently ideal situation, the atomic roughness at the tip surface still causes slight uncontrolled deviations of the ion trajectories, which presently limit the lateral resolution of the technique [4].

The situation becomes more complex if different phases at the tip surface contrast in their respective field evaporation probabilities. The threshold fields for the onset of evaporation, can differ by a factor of two or more. In response to this heterogeneity, the tip surface develops a variation of local curvature that balances the evaporation rate per surface area via an adjustment of the local surface field. Hence, the apex shape in APT experiments often deviates from the assumed hemisphere, and so significant trajectory aberrations can be observed [5,6]. In addition, the shape develops dynamically during measurement. As a consequence, imaging properties of the microscope are subject to continuous change [7], which further increases the complexity of the volume reconstruction.

Established APT reconstruction protocols are based on two premises. First, the validity of a simple ion projection law and second, the negligence of possible trajectory aberrations induced by a non-conforming tip-shape. The standard approach has been introduced by Bas et al. [8] in 1995. Except for some improvements for a wide field of view [9], this method still notably represents the accepted state of the art and is widely used by scientists working with APT [10,11]. The purely geometric approach is based on a point projection that links the impact position at the detector to

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the original position at the tip surface with a straight line. It is assumed that the emitter apex maintains a hemispherical shape during the entire reconstruction process. Only the curvature radius is allowed to change according to a presumed evolution during the measurement. The centre of the point projection is considered to lie between a stereographic and a gnomonic projection. Assuming a self-similar evolution of the emitter shape, important reconstruction parameters, the field factor and the image compression, are treated as constants, although it is well known that these reconstruction parameters undergo a characteristic variation throughout the measurement. Consequently, a variant of the standard reconstruction protocol has already been proposed to describe the reconstruction parameters as functions of the curvature radius in order to improve the quality of reconstruction in this respect [12].

The described geometric reconstruction approach is adversely affected by characteristic limitations. At interfaces between materials of strongly contrasting evaporation thresholds, densified or depleted regions as well as distortions in the geometric appearance of particles or thin films are produced [13–16]. In extreme cases, aberrations may even lead to an overlap of the trajectories of nearby atoms [17–19]. As a result, artificial zones of erroneous mixing are reconstructed. The limitations of the geometric point projection become particularly obvious in these situations.

In this work, we suggest an alternative concept for the volume reconstruction. Enabled by a recently published APT simulation package ('TAPSim' [20,21]), which is based on a flexible Delaunay tessellation, the proposed concept relies on the calculation of realistic and physically sound ion trajectories between the emitter apex and the detector entrance. To allow such an accurate calculation, the atomic order of the reconstruction must be reversed. The atoms detected last are the first to be reconstructed. The aim of this article is to outline the concept and to demonstrate its principle functionality using relatively small numeric model calculations. Before scaling the approach up to the data size of practical measurements, restrictions in computing efficiency must be overcome and the robustness of the approach against incomplete experimental data sets has to be further improved.

2. Principle of the new reconstruction approach

Imagine the arbitrary atomic geometry of the tip to be known exactly at a given moment, as illustrated by Fig. 1. It is then a straight-forward task to calculate the realistic field distribution

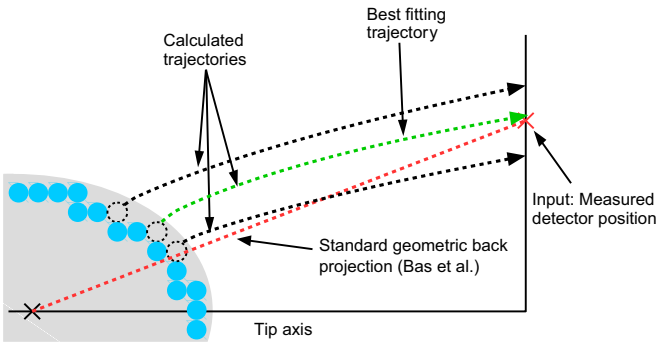

Fig. 1. Principle of the new reconstruction approach. The measured position on the detector is compared to hypothetical impact positions of calculated trajectories originating from the emitter surface. The atom is added to the tip surface at the origin of the best fitting trajectory (green). The prediction of the linear point projection (red) can be used as an estimation for the position, but is subsequently refined by the calculation of realistic trajectories. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

around the tip, if a sufficiently flexible numeric algorithm is at hand, e.g. as it has been introduced by the TAPSim package [20]. TAPSim was originally developed to simulate the evaporation of APT emitters of arbitrary structure and shape. In this study, we make use of it to maintain a realistic electrostatic model of the tip, the detector, and the field in between. In other words, TAPSim is used to refine the geometric point projection by calculation of realistic trajectories.

The basis of TAPSim is the numeric solution of the Poisson equation on a tessellation of irregular Voronoi cells [20]. Each atom of the sample structure is represented by a single Voronoi cell. Additional Voronoi cells of random geometry are used to form the bulk/vacuum interface and to fill the space between the emitter and the detector. As an important advantage, the Voronoi tessellation can be adapted to any, even irregular spatial arrangements of atoms. Furthermore, the Voronoi tessellation has a straight-forward local interpretation. The Voronoi cell around a given atom or, in general, around a given generator point, comprises all volume that is closer to the given point than to any other point of the mesh. Nearby Voronoi cells, in direct contact to the given one (distinguished by a common facet with the given cell), represent the local neighbourhood. (The generator points of these cells represent the natural next neighbours of the generator of the given cell). If at least one of the neighbour cells is a vacuum cell, the given cell obviously belongs to the emitter surface.

In TAPSim, the Voronoi tessellation is computed from its geometric dual, the Delaunay tessellation. In combination, the two tessellations give access to the potential and the electric field at an arbitrary position in space (by smooth interpolation). This enables the calculation of physically sound ion trajectories from atomic to macroscopic scale by integration of Newton´s equation of motion [22].

In the proposed concept of an improved APT reconstruction, TAPSim is used to test possible launch sites at the current emitter surface, guiding the advancing reconstruction. Trajectories, are computed beginning always at the generator point of a vacuum cell in contact to the current surface, and predicted detector hit positions are compared to the measured one. This approach sounds a bit cumbersome. The reason behind is simple: Since the velocity vector of the ion is not available in the moment it hits the detector, the trajectory cannot be calculated by back-integration from the detector to the tip surface, even if the field were accurately known. However, provided with a sufficiently good electrostatic description, it must nevertheless be possible to retrieve the original position at the tip surface. To this end, we scan possible launch sites at the emitter surface and calculate the trajectory for each case starting always with the ion at rest. The launch site for which the related trajectory best correlates with the detector event under consideration, is finally selected to place the atom into the reconstructed volume.

In order to reduce the number of trajectories to be checked, a preliminary launch position is estimated from the conventional point projection. In most cases, the trajectory calculated from this initial estimation will miss the measured impact position. Consequently, this estimate is further optimized by a directed recursive refinement of the launch position until the best match between the calculated trajectory and the measured event has been achieved. Once the new atom has been attached to its position, respective data structures of TAPSim are updated to prepare the evaluation of the next data event. I.e. the new atom becomes part of the emitter structure by modifying the content of the respective Voronoi cell. In particular, the cell is included in the set of surface cells. At the same time, cells which are no longer part of the tip surface are removed from this list. As mentioned before, the next neighbours to the surface Voronoi cells, form the set from which probable launch sites are selected. The outlined procedure is

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