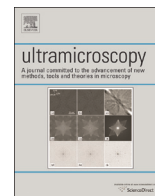




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Modeling Atom Probe Tomography: A review

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ABSTRACT

Improving both the precision and the accuracy of Atom Probe Tomography reconstruction requires a correct understanding of the imaging process. In this aim, numerical modeling approaches have been developed for 15 years. The injected ingredients of these modeling tools are related to the basic physics of the field evaporation mechanism. The interplay between the sample nature and structure of the analyzed sample and the reconstructed image artefacts have pushed to gradually improve and make the model more and more sophisticated. This paper reviews the evolution of the modeling approach in Atom Probe Tomography and presents some future potential directions in order to improve the method.

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1. Introduction

Among the usual microscopy techniques, the Atom Probe Tomography occupies a singular position. Compared to for instance X-ray imaging, neutron characterization, electron microscopy, no external beam is required to form the sub-nanometer resolved three dimensional image of the area of interest. This is the sample itself that emits and magnifies an image of its surface. The atom by atom reconstruction of this sample surface, and the elemental characterization of emitted atoms by time-of-flight mass spectrometry, produces at the end, a near atomically defined tomogram of a sub-micron [3] volume. The strength of this instrument as a microscopy tool is therefore the absence of required complicated optical devices which may limit its metrology performances. Rayleigh criteria, numerical aperture, lens aberrations, etc. are concepts non relevant in the design of a basic tomographic atom probe [1–3].

Basic physical principle of the instrument is the self-erosion of the tip produced by the effect of a huge electric field existing at the sample surface. This field, induced by the application of a high voltage to the sample prepared as a sharply pointed needle causes, first the surface atoms to be expelled by the physical process of field evaporation, and second causes the projection of ionized atoms in the electric field distribution of the tip apex. In Atom probe, ions are self-projected from the specimen onto a detector, and the property of this projection is directly ruled by the specimen. As the material surface is progressively analyzed, atom-by-atom, the projection evolves in sometimes extremely complex

ways [4]. The electric field underpins both the field evaporation process but also the projection of the ions, and any specimen surface roughness or waviness arising from non-homogeneous field evaporation induce local variations in the field distribution and therefore in magnification that cause deviations in the ion trajectory that are termed trajectory aberrations [5–7]. The experimental spatial resolution (spatial precision in a metrology point of view) of this analytical microscope was proven to achieve the atomic scale in favorable cases, a few nanometers in the worst cases [8–10]. The spatial accuracy of the image is more user-limited, depending on the recipes that are employed to rebuild the specimen from the raw data. Understanding spatial resolution limitations and improving the reconstruction recipes require a precise inspection of the tip-to-image formation mechanisms, whatever the sample and its initial shape. In this aim, for about 20 years, efforts have been pursued to model and simulate the field evaporation process in an atom probe.

This paper reviews these efforts, and presents the future advances in the modeling approaches for APT image interpretation. This paper is divided into four sections starting from a necessary description of the physical principle of field evaporation. The second section gives an overview of the general method proposed to understand the ion trajectories in Atom Probe. Some examples of recent applications of these methods are shown in Section 3. In the last section, future directions in the modeling approach are exposed.

2. Theoretical background

The controlled, atom-by-atom erosion of the sample that induces tip morphology modification, and consequently image

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formation is named field evaporation (FEV). This process is the removal of specimen atoms, in the form of ions, from the material surface, as result of the generation of a sufficient positive electric field. The aim of this section is not to be exhaustive in the consideration of the intrinsic field evaporation mechanisms but to bring sufficient understanding to build more complex modeling approaches describing the complete imaging process of atoms from its bulk position to the hit on the detector. More detailed, and less oriented reviews of this process may for instance be found in numerous books and publications [1,2].

FEV is a multistage-stage process, involving first the escape of the atom from the surface, followed then by several steps of post-ionization of the escaping particle to a final ionized state (ne the final charge of the ion). In a mesoscopic approach, the ion is rapidly accelerated in the electric field distribution produced by the polarized tip apex. Far from the tip apex (a few tens of microns ahead), the particle generally followed a straight trajectory, so that interesting features of the particle trajectory is situated in the microscopic environment of the emitter. Most of the field evaporated atoms are removed as single particles from the surface that avoid any charge-space calculations to be performed. Indeed, even at high evaporation rate, the residence time of ions is sufficiently short compared to the residence time of atoms at the surface to consider a single particle removal phenomenon.

Understanding the path of the particle from its initial position at the tip surface to the final position onto the detector, in the purpose of determining the back projection algorithm requires in principle a perfect description of the subtle movements of the atom from the very first steps of evaporation, governed by quantum mechanics theory. As we will show in this paper, any small deviations in its initial position may induce perturbation in the projected position.

Nevertheless, a fully quantum description of the evaporation process is, for the moment, far from being achievable. The level of difficulty of this approach comes from the large scale of any atom probe tip (several thousands of atoms are to be considered), the non-standard conditions to which the surface is submitted (high field physics), the fact that a time dependent approach should be required, and in a not adiabatic formalism [11–18]. In addition, any simple atom probe experiment requires thousands of atoms to be evaporated sequentially. Recent models are restrained to a few tens of atoms, where the field evaporation is calculated from selected positions at the sample surface. Results are encouraging but limited to a few cases (W, Mo, Si, Al, and some compounds), not sufficient to reveal a general behavior that may use to extrapolate to any materials.

The important results that are consistent with experiment, and offer a basis for interpretation are listed below

- Atoms are without field confined in potential well, with an adhesion energy proportional to the sublimation energy of the materials.
- Under the presence of a surface field, this well is deformed, so that an energy barrier $Q_{EV}(F)$, smaller than the adhesion energy exists and may be overcome with sufficient activation energy. Barrier crossing is achieved through a thermal process, and an Arrhenius equation can describe the rate of desorption $k_{EV}(F, T)$, with T the specimen temperature. This equation writes

$$k_{EV}(F, T) = Ae^{-(Q_{EV}(F)/k_B T)}$$

with k_B the Boltzmann constant and A the rate constant pre-factor or surface-atom vibration frequency. Note that this factor is also field- dependent.

- $Q_{EV}(F)$ decreases monotonically with F , and vanishes for a threshold electric field named F_{EV} the evaporation field of the atom.
- When crossing the barrier, the atom is rapidly ionized through a charge draining mechanism. Close to F_{EV} , the barrier maximum is situated a fraction of the interatomic spacing from the equilibrium position of the surface atom. The velocity of the atom is only temperature dependent and small considering the temperature applied (10–200 K).

It is fundamental to note that the theories that can describe or explain these processes are still in development even after 60 years of researches. The first tentative explanations were initiated by Müller and Gomer [21,22], on the basis of thermodynamic considerations. Without entering into the details (details can be found in [1] for instance), they considered the superposition of the atomic and the ionic energy curves in the presence of the field, and found the activation energy $Q_{EV}(F)$ as the difference between the atom energy level inside the well and the maximum energy level of the ionic state bent by the field (in the Müller approach) or the crossing point between the atomic and ionic curves (in the Gomer approach). In the Müller approach, the F_{EV} writes as

$$F_{EV} \sim \frac{4\pi\epsilon_0}{n^3 e^3} Q_0^2 \quad (2)$$

With

$$Q_0 = \Lambda + \sum I_n + n\Phi \quad (3)$$

Where Λ the energy corresponding to the binding energy of the atom from its site, $\sum I_n$ the sum of the ionization energy needed to create a $n+$ ion, and Φ the emitter work function. In addition, the activation energy follows in this approach a simple expression:

$$Q_{EV}(F) = Q_0 \left(1 - \left[\frac{F}{F_{EV}} \right]^2 \right) \quad (4)$$

Close to F_{EV} , this expression can be simplified to

$$Q_{EV}(F) = \frac{Q_0}{2} \left(1 - \frac{F}{F_{EV}} \right) \quad (5)$$

The agreement of these equations with experimental measurement is poor. Indeed, it is necessary to assume a high degree n of ionization in most of the case to obtain a valuable F_{EV} value. The linearity of Q_{EV} with F is experimentally observed in the range $0.8 F_{EV} - 0.95 F_{EV}$ for some materials but deviations exist out of this region. In addition the experimental estimation of $Q_0/2$ is not consistent with theoretical values. Generally data related to fractional field reduction needs to be acquired via experiment. Nevertheless, relations (2) and (5) are often used, due to their simplicity.

Another point of view can be taken if we consider not the energy that must be acquired by the atom to be desorbed (in the field free approach) but the critical force that must be exerted to an atom to be lifted out from the surface. Considering the adhesive energy diagram of an atom on the surface, that may be described by an universal binding energy curve $E(x) = D(1 + \sqrt{2}(x/l)) \exp(-\sqrt{2}(x/l))$

(or a Morse potential $E(x) = D(\exp[-2(x/l)] - 2 \exp[-(x/l)])$ [23, 24, 25, 17], with x the distance to the atom position, D the bounding energy in a pair of atoms (proportional to Λ), and l a scaling length, the maximal force that can sustain an atom is given by $F_1 \sim D/2l$. If we consider Gauss's theorem, the external electric field is induced by a surface charge layer. Surface atoms are therefore not neutral, but behave as partial-ion. An electrostatic

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