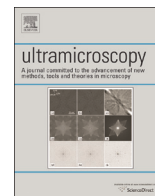




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# An analytical model accounting for tip shape evolution during atom probe analysis of heterogeneous materials

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## ARTICLE INFO

## Article history:

Received 11 September 2014

Received in revised form

5 December 2014

Accepted 14 March 2015

## Keywords:

Atom probe tomography

Tip shape evolution

Field evaporation

Simulation

## ABSTRACT

An analytical model describing the field evaporation dynamics of a tip made of a thin layer deposited on a substrate is presented in this paper. The difference in evaporation field between the materials is taken into account in this approach in which the tip shape is modeled at a mesoscopic scale. It was found that the non-existence of sharp edge on the surface is a sufficient condition to derive the morphological evolution during successive evaporation of the layers. This modeling gives an instantaneous and smooth analytical representation of the surface that shows good agreement with finite difference simulations results, and a specific regime of evaporation was highlighted when the substrate is a low evaporation field phase. In addition, the model makes it possible to calculate theoretically the tip analyzed volume, potentially opening up new horizons for atom probe tomographic reconstruction.

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## 1. Introduction

Atom probe tomography has significantly evolved since the first prototype in 1986, especially from the instrumentation point of view. Indeed, while constrained to metallic materials during the first few decades of work with APT, complex nanoelectronic device analyses are now routinely performed [1,2] with the introduction of laser pulsing [3–6] and wide field of view atom probe [7–9]. However, the standard tomographic reconstruction protocol remains very close to the original one developed at the early stage of the technique [10]. Even if attempts have been made to propose more advanced description of the specimen geometry, ions back projected onto a hemispherical surface is still at the core of the latter [11–14]. This approach has intrinsic limitations since it is well known that the shape of field evaporated end forms cannot be described so simply. Indeed, in a heterogeneous sample made up of several phases with different evaporation behavior, the evaporation sequence is highly non uniform. It results in a non-hemispherical complex surface shape, which in turns gives rise to local magnification [15]. These effects have been first postulated [16] and then demonstrated by numerical simulations [17], and they are now directly demonstrated experimentally by APT and TEM complementary analysis [18,19]. However, if great efforts have been made to model the imaging process in APT [20–23], at the moment there is no theoretical framework describing the tip

shape evolution when made up of materials with different evaporation behavior. In the current work, we propose an analytical model of the evaporation sequence in the specific case of a bilayered tip. We first derive a very general condition driving the morphology of a field evaporated surface. In a second step, we show how this condition applied to a cylindrically symmetric tip provides a full surface description. Then, based on comparison with numerical simulations, we validate the model and we highlight the origin of some field evaporation features encountered in this specific tip geometry.

## 2. Modeling

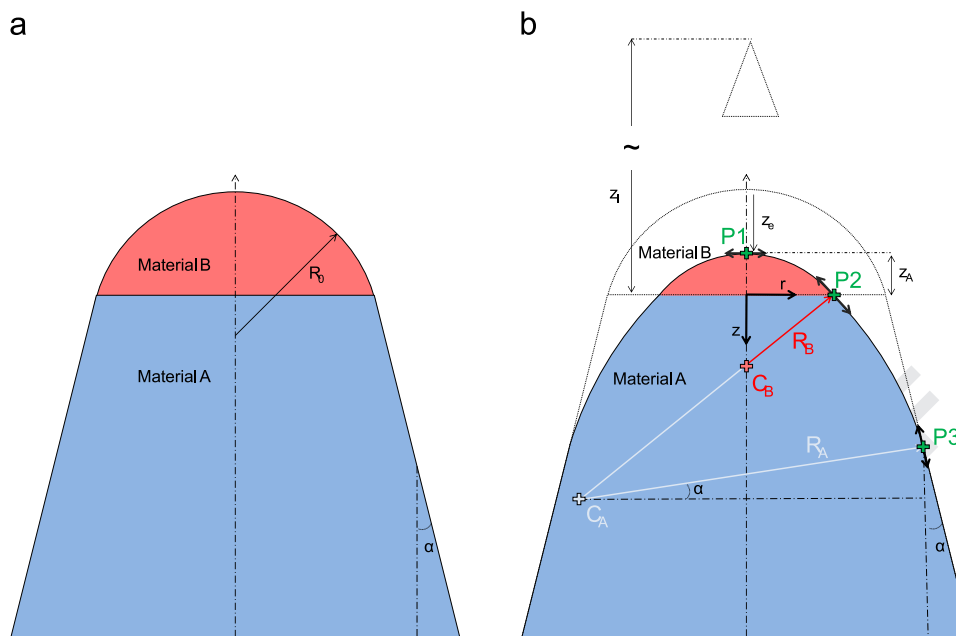
## 2.1. First regime of evaporation

The initial tip shape has been modeled by using the classical model of hemispherical cap seated on a truncated cone (Fig. 1a) [10]. The initial radius is  $R_0$  and we denote  $\alpha$  the half shank angle. The present work focuses on a tip made of an upper layer of material B seated on a layer of material A. Those layers are pure in A and B respectively, and are assumed to be perfect conductors. The A/B interface is perpendicular with respect to the z-axis, and located at the tangential point between the hemisphere and the cone.

The aim of the proposed model is a dynamic mesoscopic scale description of the apex end-form during evaporation. Field evaporation is basically an atomic scale process, involving the local atomic geometry of the surface and the chemical identity of

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**Fig. 1.** (a) Modeling of the initial tip geometry. (b) Modeling of the tip shape at the evaporation depth  $z$  in the case of a high field material B (in red) seated on a low field material A (in blue). 2 column (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

individual atoms: thus a complete picture of the phenomenon would require quantum-mechanical calculations [24,25]. Such a degree of complexity is ignored in the present paper, and the discrete positions of the surface atoms are modeled by a continuous surface. To derive the evolution of this surface, we assume the following: For a tip containing materials with low evaporation field differences, (1) the end cap forms a smooth equilibrium end shape which may be described by a continuously derivable surface, since a discontinuity of the derivative would result in non-stable atomic protrusions (2), and the field evaporation rate-constant has to be a continuous function on a smooth surface subjected to evaporation, otherwise it would also create protrusions. To complete the picture, (3) we chose to model a homogeneous phase by a constant curvature in the plane parallel to the  $z$ -axis. Fig. 1b is a schematic representation of the tip end form resulting from the model in case of a high field layer B on a low field layer A. The evaporation depth is  $z_e$  along tip axis, and layers A and B are modeled by arcs of circle (condition (3)) of radius  $R_A$  and center of curvature  $C_A$ , and  $R_B$  and  $C_B$  respectively. Condition (1) requires tangential continuity in points  $P_1$ ,  $P_2$  and  $P_3$  while condition (2) sets the ratio  $R_B/R_A$ .

The field evaporation rate-constant for the atoms at high risk of evaporation can be expressed as an Arrhenius law (we refer the reader to [9] chapter 3 for a detailed explanation of Eqs. (1) and (3)):

$$k_{hr} = A_{hr} \exp\left(-\frac{Q(F)}{k_B T}\right) \quad (1)$$

where  $A_{hr}$  is the field evaporation rate-constant pre-factor for high risk atoms,  $k_B T$  the Boltzmann factor, and  $Q$  the field evaporation activation energy depending on the local surface electric field. For atom probe analysis, the values that have to be taken into account are those corresponding to field evaporation onset, e.g. during the voltage or laser pulse. For the sake of simplicity, we make the assumption that  $A_{hr}$  is not material dependent and that the temperature is homogeneous across the whole tip apex. Now, applying the condition of continuity of the field evaporation rate-constant in point  $P_2$  results in

$$Q(F)_{P_2}^A = Q(F)_{P_2}^B, \quad (2)$$

where  $Q(F)_{P_2}^A$  is the activation energy in the close vicinity of  $P_2$  located on the material A and  $Q(F)_{P_2}^B$  is the activation energy in the close vicinity of  $P_2$  located on the material B. The field dependence of activation energy has the form:

$$Q(F) = C_l \left(1 - \frac{F}{F_E}\right)^l \quad (3)$$

where  $l$  is a constant,  $C_l$  is an energy-like parameter and  $F_E$  is the zero barrier evaporation field.

Thus:

$$(C_l^A)^{1/l} \left(1 - \frac{F^A}{F_E^A}\right) = (C_l^B)^{1/l} \left(1 - \frac{F^B}{F_E^B}\right) \quad (4)$$

$F^A$  and  $F^B$  are the electric field felt by the atoms of material A and B, close to  $P_2$ . A and B superscripts stand for “constant relative to material A” and “constant relative to material B”. Here, because we have limited knowledge about the precise surface electric field value, we are forced to introduce the expression proposed by Gomer to link the electric field  $F$  to the tip radius of curvature  $R$  [26]:

$$F = \frac{V}{k_f R} \quad (5)$$

Where  $V$  is the applied voltage and  $k_f$  is known as the field factor. We then propose to reformulate this mesoscopic formula into a local equation:

$$F(x, y, z) = \frac{V}{k_f(x, y, z) R_m(x, y, z)} \quad (6)$$

Here  $F(x,y,z)$  is the surface electric field at the point of coordinates  $(x,y,z)$ ,  $k_f(x,y,z)$  is the local field factor accounting for the tip electrostatic environment, and  $R_m(x,y,z)$  is the local mean radius of curvature. Note here that  $k_f$  is an unknown function that is sensitive to many details of the overall specimen shape and instrumental geometry: we only assume that it is not dependent on the local mean radius of curvature. Injecting Eq. (6) into Eq. (4) and

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