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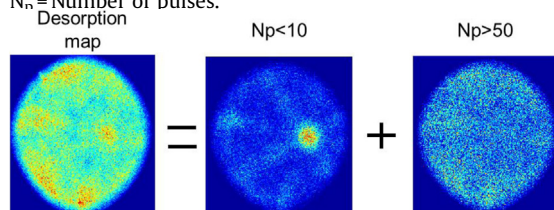
A filtering method to reveal crystalline patterns from atom probe microscopy desorption maps



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GRAPHICAL ABSTRACT

 N_n = Number of pulses.

 N_p = Number of pulses

ABSTRACT

A filtering method to reveal the crystallographic information present in Atom Probe Microscopy (APM) data is presented. The method filters atoms based on the time difference between their evaporation and the evaporation of the previous atom. Since this time difference correlates with the location and the local structure of the evaporating atoms on the surface, it can be used to reveal any crystallographic information contained within APM data. The demonstration of this method is illustrated on:

- A pure Al specimen for which crystallographic poles are clearly visible on the desorption patterns easily indexed.
- Three Fe-15at.% Cr datasets where crystallographic patterns are less obvious and require this filtering method.

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ARTICLE INFO

Method name: A filtering method to reveal crystalline patterns from atom probe microscopy desorption maps

Keyword: Atom probe microscopy

Article history: Received 9 November 2015; Accepted 23 March 2016; Available online 26 March 2016

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<http://dx.doi.org/10.1016/j.mex.2016.03.012>

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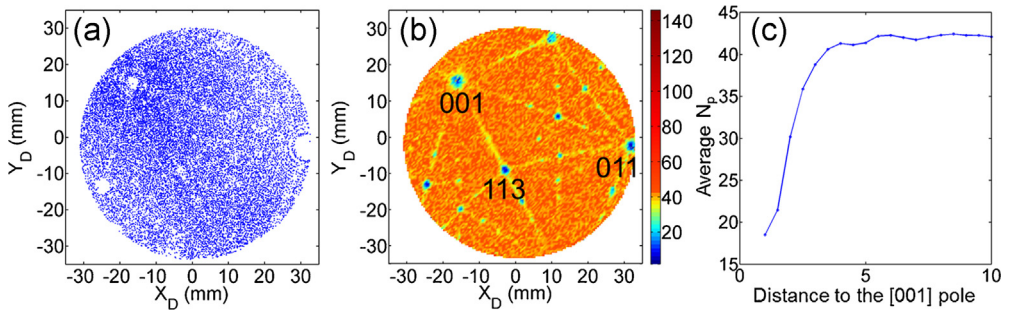


Fig. 1. (a) Desorption map of an aluminum specimen. (b) Colorized by the average number of pulses of evaporation events on each pixel. (c) Calculated distance from the [001] pole to the evaporation events classified by the average number of pulses.

Atom probe microscopy (APM) is an advanced imaging and analysis technique to acquire nano-scale chemical and structural information from solid materials with near-atomic resolution [1–3]. The collected information is presented as a 3D volume containing atoms, whose positions and chemical identities were determined. APM is the only technique providing 3D atomic-scale composition information. However the amount of structural information can often be limited by spatial resolution that strongly depends on the chemistry of the analyzed material. Field ion microscopy imaging has been traditionally used for crystallographic imaging and orientation determination of needle-shaped specimens [4,5]. However, in addition to declining popularity of this technique compared to APM, new data analysis tools have been developed to quantify crystallographic and compositional information simultaneously within APM data, which are particularly amenable for materials with relatively uncomplicated field evaporation behavior [6,7]. These data analysis techniques can not only be used to calibrate the reconstruction of datasets, or to inform on the orientation of the crystals being analyzed, but also to enable quantitative analysis of orientation-dependent features such as dislocations, precipitates, and grain boundaries [8–11].

In APM, specimens are prepared into a needle shape with a sharp pointed end. The radius of the specimen apex is normally between 20 and 100 nm. Although it is generally described as a spherical shape, the actual apex surface is not continuously smooth and presents some roughness due to the atomic nature of the surface structures. This results in the field distribution not being uniform at atomic level [12], and therefore in a non-uniform projection of the evaporated atoms onto the detector. Since the atomic surface structure directly depends on the crystallographic orientation of the specimen, the desorption maps, that are the cumulative 2D histogram of all detected atoms on the detector, can reflect the crystallinity and orientation of the sample. Low-density regions on desorption maps are generally associated with low-order crystallographic directions or planes intercepting the specimen surface, because in these regions, the surface morphology causes atoms to evaporate in directions away from the normal direction [13]. By analyzing the symmetry of the contrast patterns present in desorption maps, one may derive the crystallographic orientation of the specimen. As an example, Fig. 1(a) shows a desorption map obtained from a pure Al sample where the [001] and [011] directions can easily be identified.

Mining crystallographic information from APM datasets, however, is not always as obvious. The distinct patterns that arise from the field evaporation of pure metals or alloys with low solute concentrations come from the ordered sequence of evaporation of the surface atoms and the steady-state morphology of the surface. For more concentrated alloys, the different evaporation probability for each atom type generates randomness in the sequence of evaporation of the atoms. The departure directions of the evaporating ions becomes somewhat scattered resulting in blurring of desorption maps and crystalline patterns.

To remediate this inherent limitation, we introduce an alternative method that can be used to identify crystallographic patterns from desorption maps. During APM data collection, the field evaporation event or the time of departure of an ion from the surface field evaporation is controlled by application of voltage or laser pulses during which the evaporation rate becomes non negligible. It

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