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Origin of High-Density Zone Lines in Field Desorption Patterns of Tungsten

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Among the characterization techniques which allow us to "see" single atoms, field ion microscopy (FIM) and atom probe tomography (APT) are unique in the way that individual atoms, instead of a collection of atoms, can be imaged. At the same time, data collected by these techniques can provide three-dimensional information of atomic structures via reconstruction. Our ability to reconstruct three dimensional atomic structures however relies on our understanding of the signals. In these techniques, individual or molecular species are field-evaporated from a sharp needle shaped specimen under an intense electric field and fly towards a 2D detector where their impact is recorded. In APT, the collective impacts form a "field desorption pattern" revealing the crystallographic structure of the specimen. While the patterns reveal the crystallography and atomic arrangement with unique resolution, they are not free of artefacts.

In the desorption patterns created in APT, a number of artefacts have been reported, for example, low-density poles, high-density rings, or low- or high-density zone lines [1]. Theories such as local magnification, "aiming errors", and surface migration have been proposed to explain these phenomena [2]. In regard to the formation of high-density zone lines in APT, which are structure and material dependent, one of the popular hypotheses about their origin is the so-called "roll-up motion" [1], where atoms roll up to the top of their neighbors before they get evaporated, which however has not yet been validated. Although it is impossible to follow the single atoms during field evaporation via experiments, atoms are always trackable in atomistic simulations. Here we introduce a new simulation approach which successfully reproduces the behavior of high-density zone lines for the first time.

The simulation approach is an enhanced "TAPSim-MD" method [3] that combines the classic electrostatic field evaporation modeling approach on the basis of finite elements (FE) [4] with molecular dynamic (MD) simulations in LAMMPS [5]. This combination allows atoms in the sample tip to relax between evaporation events and integrates evaporation events as part of the MD simulation. By using net forces composed of electrostatic forces and interatomic forces, atoms are evaporated in an "ab-initio" way via MD simulation. Figure 1 shows a typical virtual tip in the case of <110> tungsten, which evolves to its steady shape starting from a cylinder.

High density zone lines observed experimentally (Figure 2(a)) are reproduced in the simulated desorption pattern for <110> tungsten as shown in Figure 2(b). Based on the analysis of nearest neighbor configurations and forces, we find that when an atom is evaporated by a moderate electrostatic force with magnitude comparable to the interatomic force, the misalignment of the two forces deviates the atom launch direction from the local field direction and causes the aberration of atom trajectories. Consequently, it gives rise to an accumulation of hit events around zone lines on the detector and forms high density zone lines. We also observe similar effects in W with different orientations, as well as other metals and can explain even more complex phenomena in intermetallic compounds and alloys.

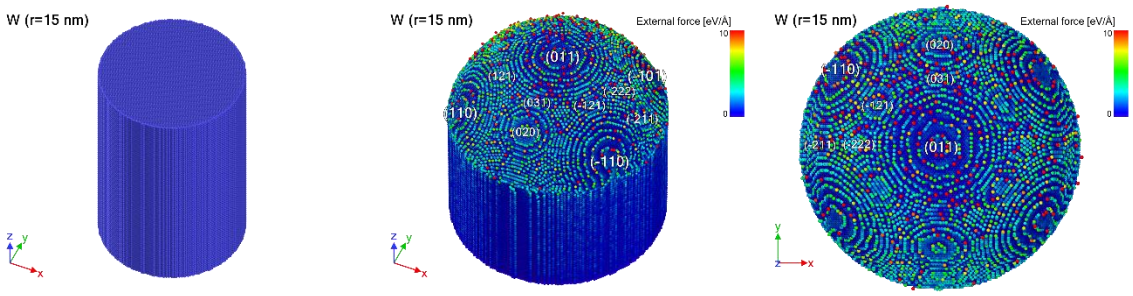

Fig 1. Simulated emitter tip of tungsten oriented in <110> direction: (a) the initial shape which is a cylinder with size of 15 nm in radius; (b) the steady-state tip; (c) the top view of the tip. The color shows the external forces during field evaporation as indicated.

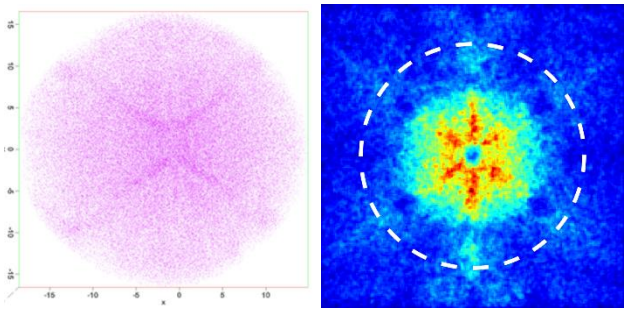

Fig 2. Desorption patterns obtained for <110> oriented W tip in (a) experiment (tip radius = 17 nm); (b) TAPSim-MD simulation (tip radius = 10 nm).

References:

[1] A Waugh, E Boyes and M Southon, Surface Science 61 (1976), p. 109.
[2] B Gault et al., Microsc. Microanal. (2021), p. 1. doi:10.1017/S1431927621012952
[3] C Oberdorfer et al., Mater. Charact. 146 (2018), p. 324.
https://doi.org/10.1016/j.matchar.2018.05.014

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[4] F Vurpillot and C Oberdorfer, Ultramicroscopy 159 (2015), p. 202.
http://dx.doi.org/10.1016/j.ultramic.2014.12.013
[5] S Plimpton, J. Comput. Phys. 117 (1995), p. 19. https://doi.org/10.1006/jcph.1995.1039
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