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Application of a Generalized Approach for APT Simulation: Investigations on Disordered and Complex Sample Structures

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Atom probe tomography (APT) is a sophisticated technique especially suited for the nano-analysis of materials composition. The analysis capabilities of the method represent the state of the art if both high spatial and chemical resolution close to the ultimate limits are demanded for materials characterization. The samples which are subjected to APT analysis have the shape of needle shaped tips. Fundamental to the technique is the extreme electric field strength (~10^{10} V/m) which develops in the immediate vicinity to the surface of these field emitter structures if a high voltage is applied. With a moderate voltage of only a few kilo volts the obtained fields are sufficient that atoms at the apex of the emitter overcome their binding to the bulk and field-evaporate from the surface. Systematic control of the generated field in combination with a fast 2D detector system and a time of flight (TOF) measurement allows collecting sufficient information to reconstruct the field evaporated volume atom by atom in a computer aided post processing step. Usual APT datasets amount to a few millions of atoms, which is equal to an analyzed volume of some 10^5 nm^3. The accuracy for the reconstructed atomic positions is best for the depth scale (~5Å) but weaker in the lateral direction (~1 nm). In the last decade the instrumentation has seen a rapid progress. Besides improved detection capabilities in particular laser-assisted field evaporation enabled the routinely analysis of insulators and semiconductors. Advanced sample preparation techniques utilizing FIB relieve from the restrictions which were due to the need of the needle-like emitter shape. Both innovations significantly broadened the range of possible assessment by APT. In contrast similar improvements have not been achieved on the “pragmatic theoretic” side. E. g. the basic reconstruction procedure still suffers from the same kind of artifacts due to local magnification effects as ten years ago. The situation becomes even worse in the case of semiconductors, ceramics etc. as the magnitude of artifacts is considered to be more severe here. In these situations electrostatic simulation of the APT measurement process provides additional information which may help to identify and interpret the impact and magnitude of artifacts.

Inspired by the former work of Vurpillot et al. [1][2], a generalized 3D approach for APT simulation [3] is presented. This new approach is founded on an irregular mesh of Voronoi (Wigner-Seitz) cells which facilitates the simulation procedure in a dual way: a) the domain associated with each single atom of the emitter structure as well as the distinct microscopic structure of the field emitter is represented by these cells, b) the geometric dual mesh of the Voronoi tessellation, the Delaunay tetrahedralization, allows for solving the general Poisson equation including dielectricity and possibly any distinguished local charge densities. This permits to fully account for the electrostatic conditions which are subjected to the emitter structure. Adaptively distributed support cells apart from the emitter additionally enable accessing the extended solution for the field covering the meso-scale.

Clearly the choice of the basic representation by Wigner Seitz-cells for the atomic structure has the basic advantage that any restrictions on the possible atomic arrangement are relieved so that structural defects as dislocations and grain boundaries, even amorphous structures are easily handled. Contrary to former simulation approaches for field evaporation, the generalized approach directly considers electrostatic forces acting on the surface atoms of the field emitter as the main criterion in order to determine the

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evaporation sequence. Figure 1 presents the example of an amorphous layer on top of a metallic substrate. The simulated evaporation of this structure was only possible with the evaporation sequence determined by the electrostatic force instead evaluating the field directly.

Most important, the possible impact of artifacts originating in lattice defects are open for investigation as physically meaningful input structures can be directly obtained from molecular dynamic (MD) calculations [4]. Figure 2 presents results for the simulated evaporation of a ∑5 grain boundary highlighting the impact of different evaporation thresholds of atoms at the GB on the reconstruction. Introduced artifacts lead to both, depletion in the reconstructed atomic density and distinguished widths for the GB in the concentration profile.

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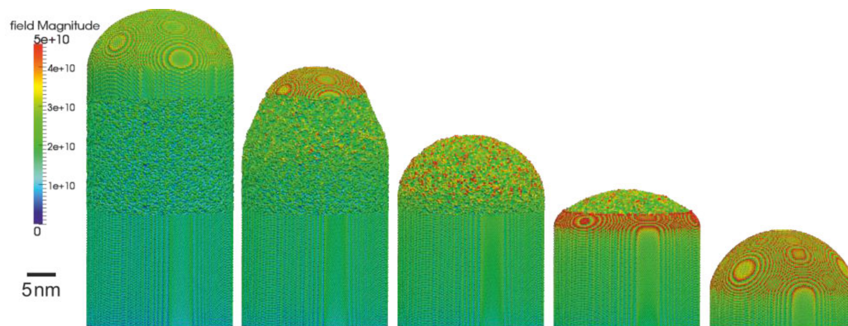

Figure 1. Snap-shots from the evolution of the emitter shape during the simulated evaporation of an amorphous structure placed on top tungsten.

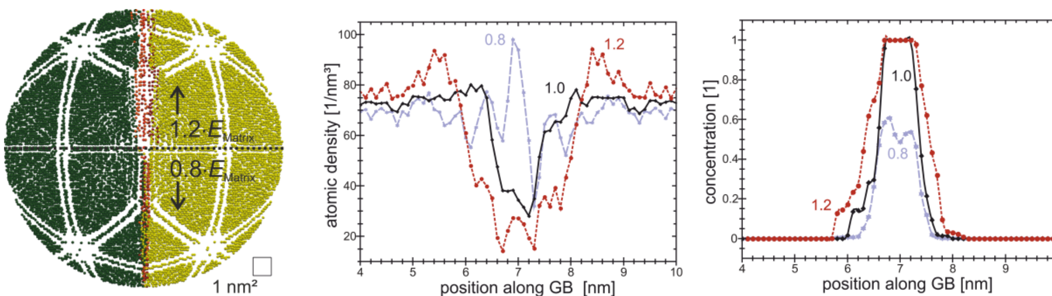

Figure 2. Simulated evaporation of a ∑5 GB. Different evaporation thresholds of segregated atoms have severe impact on the reconstructed density but also the GB width becomes affected.

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