MM 37: Topical Session Modern Atom Probe Tomography I - Fundamentals

Time: Wednesday 15:00–16:45 Location: H 0107

Topical Talk MM 37.1 Wed 15:00 H 0107

A modelling approach to understand and improve image formation in Atom Probe Tomography — •François Vurpillot, Maria Gruber, Gérald Da Costa, Alain Bostel, and Bernard Deconihout — Groupe de Physique des Matériaux, UMR CNRS 6634, Université de Rouen, BP 12 , 76801 Saint Etienne Du Rouvray, France

The understanding of image formation in Atom probe Tomography is the direct consequence of the processes of field evaporation, emission and projection of ionised atoms from the Muller field emitter (a sharply pointed needle).

Basic models of field evaporation are now more than 50 years old. The models are extremely simple and ion trajectories are known to be governed by simple electrostatic relationships. Nevertheless, because since 30 years the complexity of materials analysed with the instrument has gradually increased (from simple metals to heterogeneous materials), these simple ingredients could give rise to various image artefacts. The comprehension of these artefacts and aberrations requires the use of numerical model to improve the fidelity of image reconstruction. This paper will show how the modelling approach could be used to understand the image deformations observed experimentally in complex devices or alloys. The role of temperature will also be discussed.

MM 37.2 Wed 15:30 H 0107

Multiscale 3D Simulation Of Atom Probe Measurements — •Christian Oberdorfer and Guido Schmitz — Institut für Materialphysik, Münster, Germany

A crucial step in atom probe tomography (APT) is the computer aided post processing of the raw measurement data in order to obtain 3D elemental distribution maps. In the case of modern instruments with improved field of view and due to distinguished properties for field evaporation these maps suffer from artifacts.

The talk will address this observation by presenting recent results from computer simulations.

Main features of the presented simulation scheme are the possibility to prepare arbitrary sample structures without any constraints on distinct lattice types or lattice orientations. The representation of single atoms by Wigner-Seitz cells allows even amorphous arrangements, and, in addition, also structural defects may be incorporated.

At the same time the foundation on an adaptive mesh allows the solution of the Poisson equation covering the mesoscopic scale with suited accuracy. This way, simulated ion trajectories reflect the experimental conditions and resulting datasets become comparable to experimental ones.

Topical Talk MM 37.3 Wed 15:45 H 0107

interaction between a field emitter and an ultra-fast laser beam — •Angela Vella, Jonathan Houard, Nicolas Sevelin-Radiguet, François Vurpillot, and Bernard Deconihout — Groupe de Physique des Materiaux UMR 6634 CNRS, Universite de Rouen Avenue de l'Universite,B.P. 12 76801 Saint Etienne du Rouvray Cedex, France

In laser assisted atom probe, the surface atoms of a field emitter (nanometric tip) are ionized by the combined action of a standing electric field and an ultra fast laser to trig the emission. The tip-laser interaction causes linear and non linear optical effects but also induces a heating of the tip. The evaluation of the absorption and heating of the field emitter becomes a key factor to compare the contribution to the evaporation process of the thermal and optical effects. In this contribution, we will present experimental methods and FDTD simulations (numerical solving of Maxwell equations) to determine the absorption properties of a metallic field emitter and the resulting evaporation behaviour. The dependence of these properties on the laser beam parameters (wavelength, polarization, power) will be studied. To conclude, the differences in the optical and evaporation behaviour between metallic and semiconductor or oxide field emitter will be discussed.

MM 37.4 Wed 16:15 H 0107

Atom probe tomography of solid state ion-conductive membranes — •Gerd-Hendrik Greiwe, Frank Berkemeier, Zoltan Balogh, and Guido Schmitz — Institut für Materialphysik WWU Münster, Münster, Germany

We could demonstrate that thin film membranes of amorphous Li-borate reveal a better conductivity than quenched bulk glasses (1). We measured the Li content by atom probe tomography. Layers of Li-borate and Li-silicate glasses were deposited upon tungsten tips. Although complex, the mass spectra are well understood in terms of various molecular species allowing a quantitative analysis. New effects at the interfaces were observed, that can be explained with the dielectric and ion-conductive properties of the glasses. By applying a base voltage to the specimen during the measurement, we create an electric field over the glass layer. Mobile Li ions redistribute to compensate the field. Therefore, we measure increased Li concentration at the surface and a depleted zone at the layer/substrate interface.

Using a model of field penetration and band bending by Tsong (2) we calculated the resulting electric field in the layers and its effect on the diffusion of the Li ions. This model predicts a field penetration of a few angstroems, forming a space charge surface layer. The calculations show reasonable agreement with the measurements, thus confirming the model.

(1) F. Berkemeier, M.R. Abouzari, G. Schmitz, Ionics, 15 (2009) 241
(2) T.T. Tsong Surface Science 82 (1979) 28-42

MM 37.5 Wed 16:30 H 0107

Investigation of optical properties of Silicon under high electric field by atom probe tomography — •Laurent Arnoldi[1], Angela Vella[1], Nicolas Sevelin-Radiguet[1], Francois Vurpillot[1], Tatiana Itina[2], Elena Silaeva[2], Nikita Shcheblanov[2], and Bernard Deconihout[1] — [1]Groupe de Physique des Matériaux, France — [2]Laboratoire Hubert Curien, France

In laser assisted atom probe, surface atoms are emitted from a tip in the form of ions by the combined action of an electrostatic standing field and a laser pulse that triggers the emission. The absorption of the light by the tip apex generates a pulse heat. Models have been proposed to explain the laser tip interaction and to evaluate the temperature rise and it spatial distribution on the specimen. In this contribution we will focus on the interaction between a silicon tip and an ultra-short laser pulse. New experimental methods to determine optical properties of the field emitter in real analysis conditions (very high electric field, cryogenic temperature) will be presented. Numerical solving of Maxwell equations allow predicting the changes of the tip's absorption when the illumination conditions are modified. These simulations incorporate the refractive index of the tip surface as derived from the calculation of the band bending effect on the surface that increases the density of free careers in the presence of the field. By comparing these simulations and experimental results, we will show that the absorption of a subwavelength tip is strongly dependent on the standing electric field applied to the sample.