doi:10.1017/S1431927617003853
Microsc. Microanal. 23 (Suppl 1), 2017

Recent Reconstruction Developments in IVAS

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As part of the APTITUDE [1] collaboration we have pursued several paths for atom probe tomography (APT) reconstruction improvement. In terms of evaporation simulation, we have commercialized the 2D evaporation simulation, Figure 1a, developed at Groupe de Physique des Materiaux (GPM) [2]. In addition to simulating the evaporation physics of azimuthally symmetric specimen models, this tool also includes a graphical interface for programming geometric and evaporation parameters as well as illustrating calculated field strengths and particle trajectories.

We have taken a first step towards multimodal imaging registration by implementing a planar landmark registration reconstruction, Figure 2. This was inspired by the GPM development based on using isosurfaces during the projection phase of the reconstruction. In our implementation, we first do a complete spherical reconstruction and then perform the planar landmark registration deformation in position file (*.POS) space. Our current implementation allows the co-registration of multiple interfaces of different composition definitions. We have the capability to: force interfaces flat, force flattened or unflattened interfaces to be parallel, and to force smoothed or unsmoothed interfaces to be at specified displacements from another specifc interface. Diagnostic pseudo-POS volumes (described below) are generated that illustrate the 3D displacements that were applied during the registration deformation.

As part of the development of the landmark registration technology we found it useful to implement several improvements to our interface analysis tools. The Fourier delocalization was improved to reduce noise, and arbitrarily orientable clipping planes are now exposed on cubic regions of interest, Figure 1b . To improve the robustness of interface definitions when used for landmark registration we have also implemented a "healing" technique that can fill interface holes.

To quickly visualize the multiple 3D composition volumes that are used to compute the isosurfaces we have introduced a multi-channel volume renderer. This is similar to the opacity volume render that was already available in IVAS® but now has the capability for integrating the contributions from multiple species simultaneously.

One of the primary parameters necessary for APT reconstruction is the lateral magnification. We have historically used the image compression factor (ICF). Methods for determining the ICF have been described using crystallographic patterns in detector event maps exhibiting pole artifacts [3]. IVAS now includes a feature based on the EDAX™ OIM® tool that automatically finds and indexes poles in crystallographic images [4], Figure 1c. We use this technique to present an automated image compression factor determination procedure, Figure 1d

To make the selection of reconstruction parameters more deterministic we have begun to implement reconstruction quality metrics. One approach we are currently investigating is variability in relative density. To this end, we have developed tools that can be used to reassign the mass values of ions in a POS file with their neighborhood relative density. Tools that will be also described perform log conversion of the metric values in these pseudo-POS files and automatically generate RRNG files with programmable colormaps. Software can then be used to visualize both the statistical distribution of relative density metrics, as well as, the per-ion 3D distribution of metric values. Similarly, the same tool-chain can be used to interrogate the distribution of charge-state ratios.

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[1] The authors acknowledge funding from the Recherche Technologique de Base (RTB) and the French National Agency (Project no. APTITUDE ANR-12-NANO-0001).
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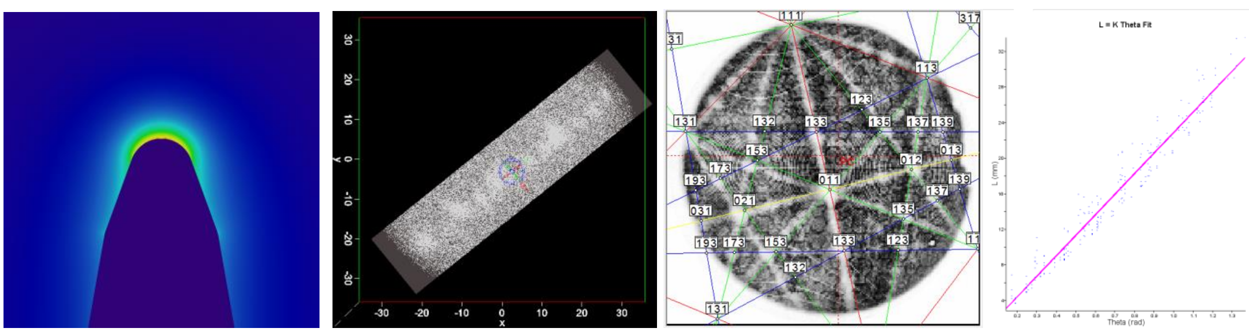

Figure 1. a) 2D evaporation simulation, b) arbitrary clipping planes, c) automatic pole identification with OIM, d) image compression factor calculation.

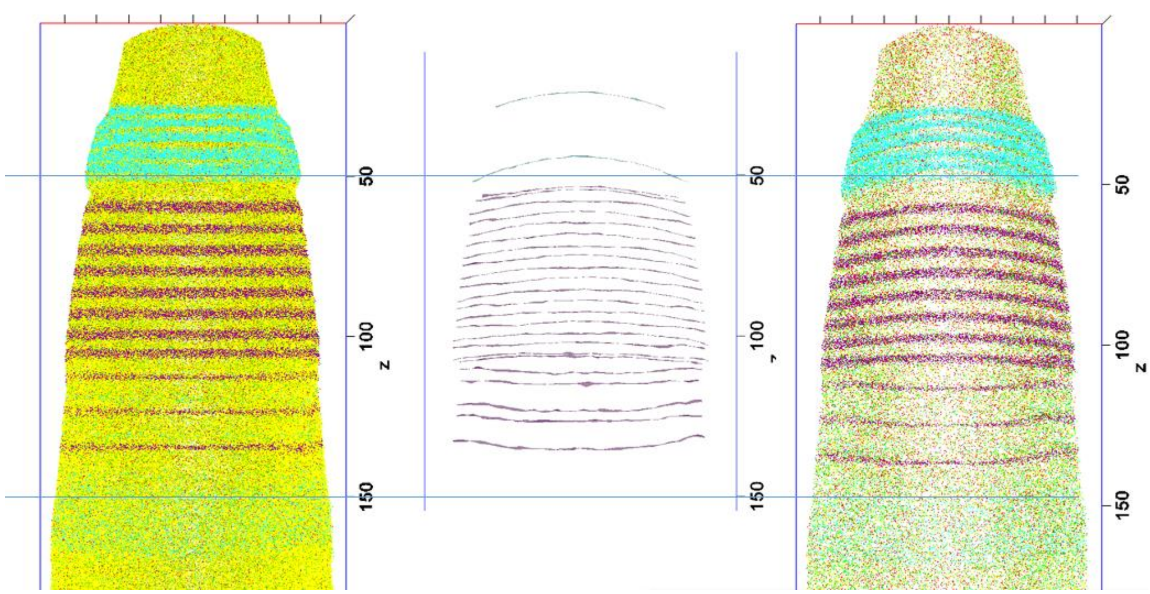

Figure 2. Planar landmark registration of multiple isosurfaces. Al8%, In3% and In0.7% isosurfaces were used.

https://doi.org/10.1017/S1431927617003853 Published online by Cambridge University Press