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Multi-modal, scale bridging analytics in energy research

Energy systems like solarcells, fuel cells and batteries contain a variety of different atoms from all over the periodic system, thereby attributing to strongly varying materials and device properties. The materials are usually stacked in layers of varying thickness and are composed of micro- or nano-particles or consist in grains and phases embedded in complex matrix materials. All components contain a wealth of interfacial area which has tightly to be controlled for optimized performance. Our goal in energy research is to control material properties at all scales from macro to atomic scale and to optimize materials in a tight feedback loop with device manufacturers who optimize and control device performance. In this endeavor, control needs to be taken over composition, grain and particle sizes, interfacial properties, defect population, topological, electrical, mechanical, optical and compositional properties. In our lab in Forchheim, Nuremberg Metropolitan Area, Germany, which is built as a joint venture of the Fraunhofer Institute for Ceramics Materials and Systems – IKTS and the Institute for Nanotechnology and Correlative Microscopy – INAM and which profits from the labs@location status with Carl Zeiss Microscopy and the strategic demo-site collaboration with Leica Microsystems, Horiba Europe/Scientific, Park Systems and Photon Energy, we established a preparative workflow (Fig. 1) for energy materials which includes an inert transfer line from a glovebox over cutting, grinding, polishing and ion-milling steps all the way into microscopes and spectrometers as much as a cyro-workflow where needed, e.g. during ion-milling and electron microscopy. The analytics (Fig. 1) include imaging with electrons, ions, x-rays, light and probes in 2D and 3D (tomography) as well as spectroscopy (mass, Raman, infra-red) at length scales from macro to nano together with mechanical and topological testing as well as electrical, optical and compositional analysis. The underlying multi-modal, scale-bridging data will be analyzed correlatively and quantitatively with the help of the nanoGPS technology [1] and powerful database systems (KnowitallR) as well as workflow engines such as the XamFlowR platform powered by Lucid concept [2] and image recognition software powered by machine learning algorithms and statistical data evaluation tools. This analytics lab will be used to study even the most delicate energy materials comprehensively to give guidance to device optimization and to contribute with data to the creation of a digital twin.

References

[1] https://www.horiba.com/deu/scientific/products/detail/action/show/Product/nanogps-navyx-4959/
[2] https://www.lucid.ch/

Figures

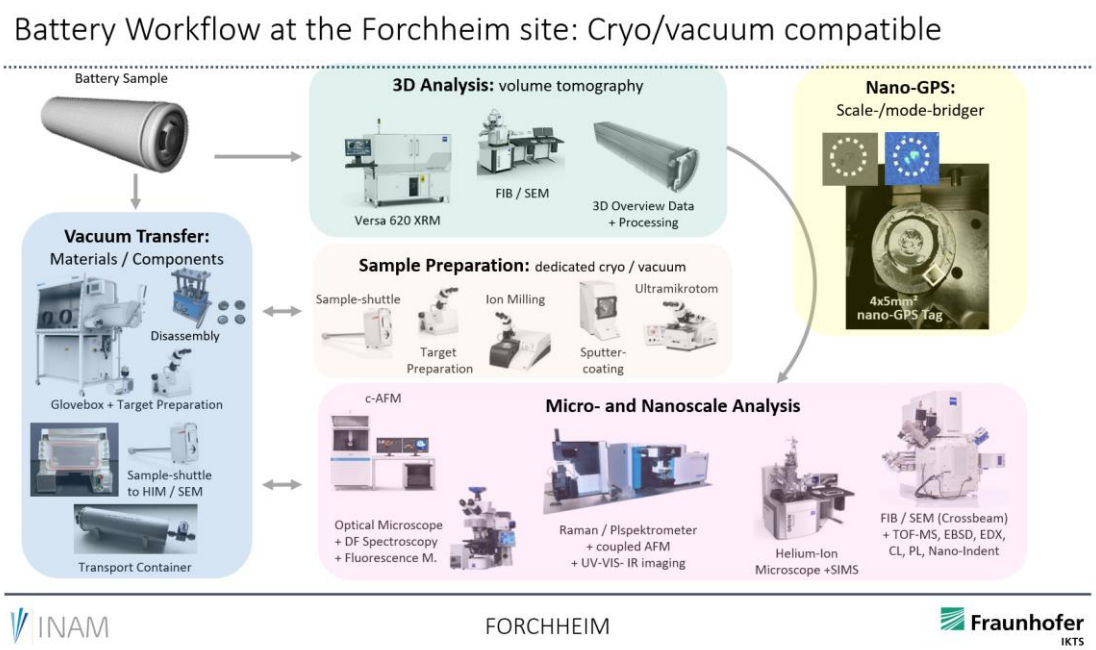

Figure 1: Battery workflow from inert sample preparation and sample transfer, scale bridging, multi-modal micro- and nanoscale analysis and the nanoGPS technology [1] as an enabler for true data correlation at the nanoscale.