In-situ meets operando meets multi-modal:Latest Developments in X-Ray Microscopy for Solar Cells

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We present the latest developments in the solar cell characterization by X-ray microscopy with respect to novel techniques, analysis methodologies, and applications. We give an overview of the developments that are driven by the achievements on X-ray source, and demanding experiments based on three examples.

First, we highlight advances in electrical characterization: with the development of the X-ray beam induced voltage (XBIV) measurement technique and the introduction of lock-in amplification for highly sensitive X-ray beam induced current (XBIC) and XBIV measurements, the full current-voltage dependence of solar cells has become accessible at unprecedented nanoscale resolution. We demonstrate applications for a variety of solar cells including Cu(In,Ga)Se_2, CdTe, and perovskite absorbers. Beyond the standard correlation of the electrical performance with elemental composition at the nanoscale, we observe inhomogeneities of the temperature-coefficients of solar cells that are operated close to outdoor conditions, by nanoscale feature tracking of industrial solar cells.

Second, we discuss applications of a dedicated heating stage for in-situ and operando measurements at scanning nanoprobe beamlines. We show results of Cu(In,Ga)Se_2 semiconductor growth in-situ from metallic precursors (Cu, Ga, In, Se) based on scanning X-ray fluorescence measurements at 600 °C. We observed not only the evolution of different phases up to the formation of Cu(In,Ga)Se_2, but were also able to extract molar fluxes and found that Cu is the driving element.

Third, we discuss scanning nanoprobe experiments where we measured simultaneously the strain distribution within Cu(In,Ga)Se_2nanocrystallites in the solar cell absorber through XRD, the local performance through XBIC/XBIV, and the elemental composition through XRF. These measurements are related to nano-XRF tomography measurements of the elemental distributions within a crystallite. We found a positive correlation between strain and performance, which points to strain engineering as worthy of further consideration.

We emphasize the need for simultaneous assessment of spatially resolved performance (operando) with structural and compositional information (multi-modal), while the device operates in the desired environment (in-situ). Through the combination of operando, multi-modal, and in-situ measurements, we make sure that we address not only scientifically interesting but also societally relevant knowledge gaps.

Particularly, the multi-modal approach that allows direct pixel-by-pixel comparison of different parameters demands sophisticated analyses to extract a maximum of information from the large data sets. We demonstrate our approaches of machine-learning techniques beyond standard statistical methods.

Such multi-modal measurements are challenging on different levels. Therefore, we discuss limitations of current synchrotron beamlines, and give an outlook to future measurements that will be enabled by Gen IV storage rings and X-ray free electron lasers.