## From the surface into the bulk: Scanning probe microscopy on Cu(In,Ga)Se<sub>2</sub> solar cells

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Alkali-fluoride (AlkF) post-deposition treatments (PDT) have led to significant increases in the power conversion efficiency of polycrystalline Cu(In,Ga)Se2 (CIGSe) solar cells. Nevertheless, а full understanding of their role and impact is not yet established. We used Kelvin probe force microscopy (KPFM) to investigate the local electronic properties of grain boundaries (GBs) for CIGSe absorbers with different AlkF-PDTs. The results show a strong difference in the potential variation across the GBs for samples with different alkali fluorides, which correlates with the open circuit voltage of reference solar cell devices. The findings suggest that heavier alkali lead to better passivation by reducing the density of charged defects at GBs [1]. However, these results rely on surface potential information collected at the surface of the AlkF-PDT CIGSe, and the electronic structure of grain boundaries in the bulk remains unknown [2]. Here, we explore the nano-scale electronic properties of CIGSe absorbers into the bulk of the layer, by using an emerging conductive atomic force microscopy (C-AFM) tomography method. Highly-doped diamond-coated AFM tips are scanned repeatedly across the same area using high tip-load forces of several µN, leading to а tip-induced material removal [3.4]. Simultaneously, the local tip-sample current is recorded. The layer-by-layer C-AFM images (Fig. 1a) finally result in a 3D current volume (Fig. 1b), reaching deep into the bulk of the CIGSe layer.

We present how the C-AFM current signal depends electronic properties such as doping on concentration, bandgap, and electron affinity. Furthermore, we developed a methodology for the quantitative analysis of the C-AFM current signals, in consistency with a mechanical model describing the materials removal. The analysis enables to determine the charge-carrier concentration of individual grains in the polycrystalline CIGSe absorber. For CIGSe with various AlkF-PDT treatments, we find that a lower efficiency solar cell with a KF-PDT shows a stronger inhomogeneity of charge-carrier concentration, while RbF and CsF lead to narrow distributions at higher charge-carrier concentrations. The charge-carrier concentration and its homogeneity relate directly to the opencircuit voltage of solar cell devices, thereby impacting the device performance. Thus, the success of the AlkF-PDT can be hampered by spatial inhomogeneities in the charge-carrier concentration. Furthermore, analysis of grain

boundary currents reveals that they behave similar in the bulk to what is observed near the surface.

## References

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## Figures



**Figure 1.** C-AFM tomography on non-PDT CIGSe. (a) Left column: Selected scans of the topography ( $20 \times 20 \mu m2$ ) at different stages of the tomography experiment, showing the evolving hole milled with the AFM tip. Right column: Corresponding current maps inside the tomography area ( $10 \times 10 \mu m2$ ). (b) 3D representation of the extracted C-AFM tomography current volume ( $10 \times 10 \times 1.8 \mu m3$ ), indicating the analyzed area for the current depth profiles of various grains.