

Visualization of the impact of RbF(S) PDT on state-of-the-art CIGS grains by cathodoluminescence

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Power conversion efficiencies of polycrystalline thin films PV technologies are boosted by post deposition treatments (PDT). These PDT involve annealing in the presence of heavy extrinsic elements like alkali-fluoride in the case of CIGS. While much is known on the role played by these PDT on the macroscopic electronic properties or even on diffusion of chemical elements^{1,2}, there is still a lot to learn on their influence on optoelectronic properties at the microscopic scale, in particular at the grain level.

Here, we investigate the role of RbF PDT performed under S atmosphere on state-of-the-art CIGS thin films. First, we quantified the impact of the PDT on the optoelectronic properties of solar cells (V_{oc} , J_0 , $n...$), see Fig. 1(a), and we conclude on a lower non-radiative recombination rate after the RbF(S) PDT as compared to the reference sample, despite their similar dominant recombination activation energy (deduced from $V_{oc}(T)$ extrapolation). Then, we analyse the impact of the PDT at the nanoscale to dissociate its influence on the grains interiors (GI) and the grain boundaries (GB) using high resolution cathodoluminescence (CL) mapping at room- and low-temperature.

Figures 1(b,c) show panchromatic room temperature (RT) CL maps, where we were able to clearly distinguish the contribution from GB and GI. From panchromatic RT CL profiles, we observe a clear increase in the radiative efficiencies in GIs. Then, low temperature (LT) hyperspectral CL maps display an inhomogeneous peak position between grains and a blueshift of the CL peak position from the GB to the GI (Fig. 1(d,e)). Besides, defects passivation within grains is observed when the PDT is applied to the materials.

We were able to conclude on the crucial role played by RbF(S) PDT on the bulk properties. The increase in the V_{oc} can be explained by both a defects passivation and/or an increase in the doping level in grains. This result can be attributed to a diffusion of species during the PDT from GB to the GI allowing for a passivation of defects or an increase of the doping level within grains.

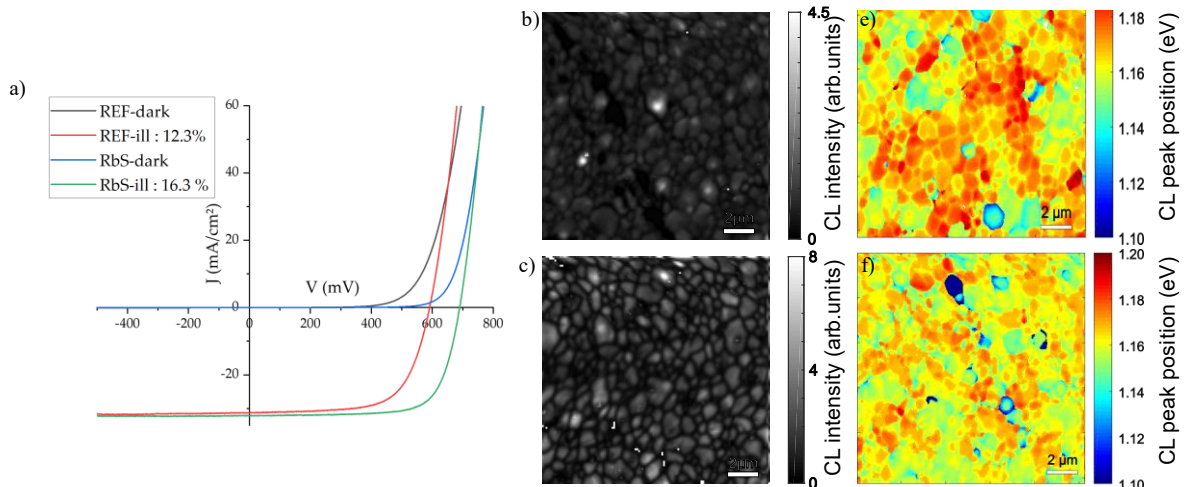


Figure 1: a) dark and 1-sun I-V curves of CIGS reference and RbF(S) treated samples. b) c) panchromatic RT CL maps (128*128 pixels) of b) ref and c) RbF(S) treated samples. d) e) LT CL peak position of d) ref and e) RbF(S) treated samples.

1. Rusu, M. *et al.* Electronic Structure of the CdS/Cu(In,Ga)Se₂ Interface of KF- and RbF-Treated Samples by Kelvin Probe and Photoelectron Yield Spectroscopy. *ACS Appl. Mater. Interfaces* **13**, 7745–7755 (2021).

2. Schöppe, P. *et al.* Overall Distribution of Rubidium in Highly Efficient Cu(In,Ga)Se₂ Solar Cells. *ACS Appl. Mater. Interfaces* **10**, 40592–40598 (2018).