## High-resolution cathodoluminescence on polycrystalline CdSeTe for photovoltaics: the role of selenium

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Polycrystalline Cadmium Telluride (CdTe) thin-film solar cells have a very low levelized cost of energy and provide an attractive alternative to Si cells. Over the last ten years, despite an efficiency hindered by the presence of defects in grain interiors and at grain boundaries (GB), CdTe solar cells have benefited from numerous discoveries improving their efficiency from 16.7% to 22.1% [1]. The latter record was driven by the incorporation of Selenium compositional grading in the layer. It shows a significant rise of the short-circuit current by bandgap lowering, with a decrease of the open-circuit voltage deficiency [2]. The excellent optoelectronic properties are attributed to the Se alloy that passivates bulk defects and GBs [3,4]. Yet a complete and quantitative physical understanding is still missing.

In this work, we present a systematic study of CdSeTe cells with various Se concentration (CdSe<sub>x</sub>Te<sub>(1-x)</sub>, x from 0 to 0.4). High spatial resolution cathodoluminescence (CL) mapping performed at room- and low-temperature on the same area allows us to quantify the passivation role of Se. We demonstrate that the radiative efficiency depends only on the peak position (Se concentration): a ten-fold enhancement is measured between x=0 (CdTe) and x=0.4 samples. CL is used to map polycrystalline CdSeTe films (CdCl<sub>2</sub> annealing) (Fig.1(a,b)) : each spectrum is fitted with the generalised Planck law coupled to a proper absorption model [5] (Fig.1(e)) in order to link the bandgap energy to the Se concentration. Selenium content maps have been extracted for each sample (Fig.1 (c,d)), revealing a preferential Se diffusion along CdTe grain boundaries : the diffusion coefficients of Se atoms along grain boundaries is found to be 8-times larger with respect to grain interiors [6].



**Figure 1:** Panchromatic maps of CL intensity for  $CdSe_xTe_{1-x}$  samples with nominal Se content of x=0.2 (a) and x=0.4 (b) along with the corresponding Selenium concentration maps (c,d). (e) Normalized CL spectra averaged over the area shown as colored rectangles in panels (a) and (b)(solid lines). Dashed lines correspond to the generalized Planck law fit, open circles on the CL spectra indicate the bandgaps determined from the fit.

- [1] M. A. Green *et al.*, "Solar cell efficiency tables (2021)
- [2] J. D. Poplawsky et al., Nat. Commun., 7, 1–10, (2016)
- [3] T. A. M. Fiducia et al., Nature Energy 4, 504-511, (2019)

[4] T. A. M. Fiducia et al., *Solar Energy Materials and Solar cells*, **238**, 111595, 2022

- [5] H.-L. Chen, et al, Phys. Rev. Applied, 15, 024006 (2021)
- [6] B. Frouin, T. Bidaud, et al., manuscript in preparation