Simulated perovskite degradation mechanisms and impact on opto-electrical performances

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Perovskites solar cells have reached high power conversion efficiencies, and improving their stability is now a major concern. Measurements of their optical and electrical performances along time are frequently used to quantify their degradation [1]. However, mechanisms can be numerous and have varying reactions rates depending on temperature, humidity, illumination or applied voltage [2]. This work aims at determining the cause of experimentally measured degradation and focuses on current-voltage characteristics (IV curves) and photoluminescence (PL) spectra.

First, initial performances of the studied device are reproduced. A statistical approach is used since some characteristics are not precisely known for each fabricated solar cell. In fact, carrier mobilities, defect densities in each layer and at interfaces depend significantly on the fabrication conditions.

This provides a basis to implement several degradation mechanisms and quantify their impact on IV curves and PL spectra. Figure 1 A. and B. show the evolution along one example. Considering both characterization techniques allows to distinguish various mechanisms. In the example, deep defects are considered: the impact is mainly an increase of Shockley-Read-Hall (SRH) recombination. However, formation of shallow defects can be distinguished through the enhancement of sub-bandgap absorption, modifying the photoluminescence spectrum in the low energy range [3].

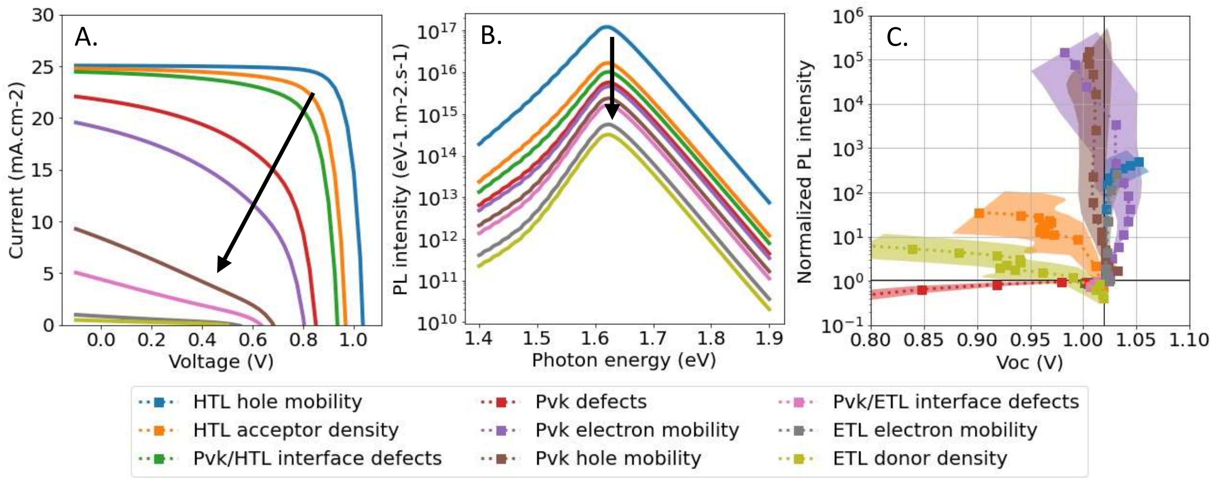

Figure 1: A. and B. Current voltage curves and photoluminescence spectra simulated for an example degradation mechanism: increasing defect density in perovskite layer. C. Degradation pathways in terms of total PL emission versus Voc for nine degradation mechanisms. Shaded areas display the confidence interval around the average pathway (squares and dotted lines), stemming from the statistical approach.

Finally, evolutions of simulated and experimental IV curves and PL spectra are analyzed in terms of correlation pathways as showed in Figure 1 C. (Numerous parameters are extracted: Voc, Jsc, FF, series and shunt resistances, PL maximum wavelength, total emission, PL spectrum slopes, width at peak half height, etc.). This avoids the time dependence of the results and associated activation effects: they are "intrinsic" characteristics of the mechanisms and independent from measurements conditions. As a result, the experimental pathway is compared to the simulated ones, and the closest has most probably caused the measured degradation.

This work tackles the causality of degradation mechanisms on perovskite solar cells performances, by simulating their optical and electrical behavior. It provides a novel way to analyze experiments, that can confirm or question interpretations from other characterization methods, that mainly grasps the correlation of degraded materials with diminished performances.

[1] M. V. Khenkin *et al.*, "Consensus statement for stability assessment and reporting for perovskite photovoltaics based on ISOS procedures," *Nat. Energy*, vol. 5, no. 1, pp. 35–49, 2020.

[2] C. C. Boyd, R. Cheacharoen, T. Leijtens, and M. D. McGehee, "Understanding Degradation Mechanisms and Improving Stability of Perovskite Photovoltaics," *Chem. Rev.*, vol. 119, no. 5, pp. 3418–3451, 2019.

[3] N. Falsini, G. Roini, A. Ristori, N. Calisi, F. Biccari, and A. Vinattieri, "Analysis of the Urbach tail in cesium lead halide perovskites," *J. Appl. Phys.*, vol. 131, no. 1, p. 010902, 2022, doi: 10.1063/5.0076712.