Analysis and Modelling of Recovery Mechanisms in Perovskite Solar Cells

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For the last decade, perovskite solar cells have attracted increasing attention from the photovoltaics community due to the improvement of their power conversion efficiency and low fabrication costs. This presents a window of opportunity for this technology to be rapidly deployed in the photovoltaic market. However, their stability still remains a challenge [1] and it needs to be properly understood to obtain reliable perovskite solar modules. While long-term degradation mechanisms have been progressively studied by the scientific community, limited research on performance recovery has been conducted and there is still a lack of comprehension of the physical rationale behind it.

To understand recovery mechanisms, experimental devices synthesized and characterized at IPVF have been modelled. Drift-diffusion and transfer-matrix methods are used to simulate optoelectrical characteristics, and a genetic algorithm has been developed to reproduce the initial performances of solar cells, based on a statistical approach. Recovery mechanisms are simulated by varying a single material parameter, such as defect density or carrier mobility in a given layer. Evolutions of correlations between optoelectric parameters are obtained, as shown in Figure 1(a). Simulated pathways are time-independent, which avoids modelling activation processes related to environmental conditions such as temperature, illumination, humidity, or applied voltage. Thus, they are very useful for identifying relevant mechanisms: each pathway is a signature of recovery describing the states that the device undergoes.

Recovery pathways are simulated and compared with those obtained from experimental periodic current-voltage measurements performed during aging, and feasible mechanisms governing recovery can be selected or discarded. This is applied to two different lots of devices fabricated and characterized at IPVF. For the first, long-term degradation and recovery during light-soaking regimes are observed during aging. Results on Figure 1(b) show that defects in the bulk perovskite layer play a key role in both recovery and degradation. Also, interfaces have a relevant impact on recovery, especially the ETL. Aging of the second lot shows a degradation trend followed by recovery only for non-passivated devices. Deep defects in the perovskite are relevant again. In addition, the variation of hole mobility in the perovskite is important for non-passivated devices, while the reduction of doping in the ETL is identified for the degradation of the non-passivated. Finally, subfamilies of the simulated mechanisms are obtained by means of clustering with machine learning techniques, gaining insights into physical parameters that better explain the experimental behavior of the devices.

Overall, this work provides new insights into recovery and degradation of perovskite solar cells. Mechanisms impacting the devices during light soaking, recovery, and degradation are identified. Thus, the reversibility of these mechanisms can be assessed, allowing to focus experimental efforts on irreversible degradation, which is more detrimental to the solar cell's stability.

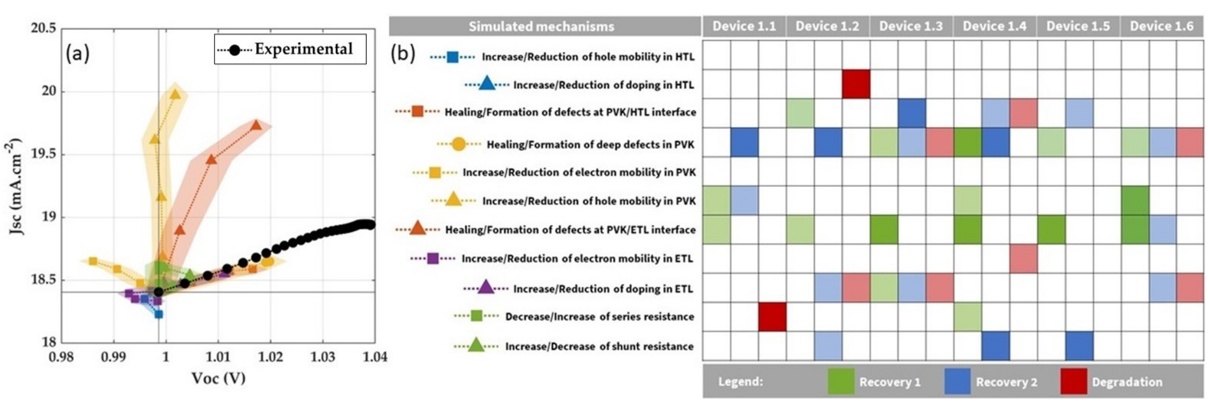

Figure 1: Identification of recovery mechanisms. (a) Correlation pathways of a single recovery. (b) Summary of results. Device fabrication methods vary precursor preparation day and solution preheating before deposition. Color intensity represents simulated mechanism status - opaque: dominant, translucid: relevant, empty: non-relevant.

[1] Caleb C. Boyd, Rongrong Cheacharoen, Tomas Leijtens, and Michael D. McGehee, *Understanding Degradation Mechanisms and Improving Stability of Perovskite Photovoltaics*, *Chemical Reviews*, vol. 119, no. 5, pp. 3418-3451, 2019, DOI: 10.1021/acs.chemrev.8b00336