Simulation of perovskite degradation mechanisms and interpretation of experimental results

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Perovskites solar cells are promising candidates to provide highly efficient and easy to produce devices. Despite performance improvements obtained in recent years, the main issue remains their stability[1]. Moreover, it is often difficult to distinguish and understand the mechanisms involved in the degradation of such devices. Degradation experiments often consist in measuring the decrease of cell efficiency with time and the evolution of electrical parameters such as output power, open circuit voltage, short circuit current or full current-voltage characteristics[2]. Time-dependent behavior can be however difficult to interpret, as degradation mechanisms can be numerous and have varying reactions rates even depending on temperature, humidity, illumination or applied voltage. Here results are analyzed without having to interpret time dependence, by plotting short circuit current density (Jsc) against open circuit voltage (Voc) and shunt resistance (Rsh) against series resistance (Rs). Drift-diffusion simulations are used to investigate the impact of the deterioration of several material parameters such as defect densities, or carrier mobilities in the different layers of a perovskite solar cell. Furthermore, several perovskite reference devices with different material properties are subjected to the same chosen degradation mechanisms. Batch simulations are performed with SCAPS 1D, each corresponding to a given degradation mechanism, for a given device. Current voltage characteristics are extracted and fitted with a single diode model Results show that the behaviors for the same mechanism and different devices are similar in the selected representations, the average and standard deviation are computed and represented in Figure 1 in colors.

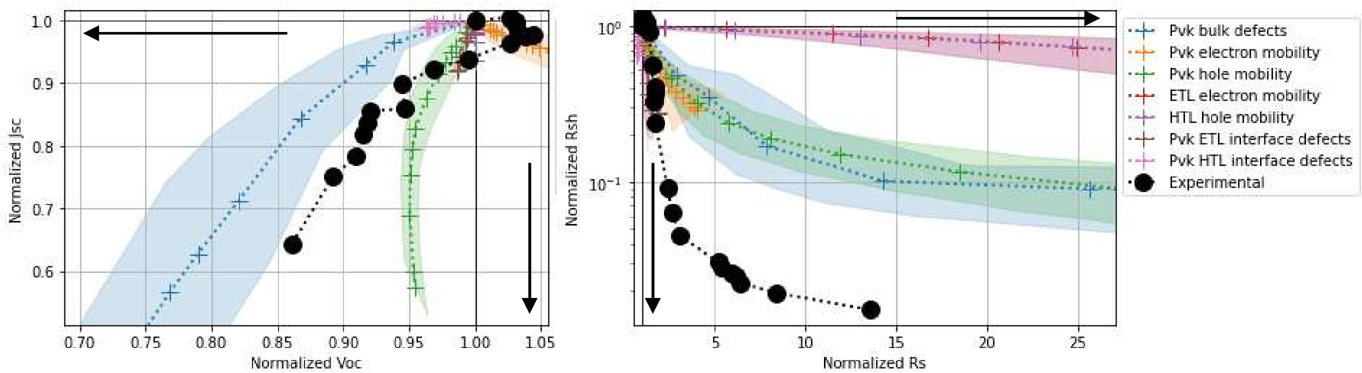

Figure 1: Correlation of Jsc/Voc (left) and Rs/Rsh (right) for seven degradation mechanisms. Average value over all perovskite reference devices is represented with crosses and dashed lines, shaded areas represent the standard deviation. Plain dark circles show perovskite experimental data from Lim et al*. 2021.*

Furthermore, perovskite experimental degradation data from Lim *et al.* 2021 are represented in the same manner and showed in Figure 1 as well. It appears that experimental Jsc/Voc data (left) show a behavior located between the ones associated with bulk defect formationandloss of electron mobility in the perovskite layer. Similarly, the same two mechanisms are the most similar on Rsh/Rs graphs (right). On the contrary, mobility losses in extracting layers do not cause a strong variation in shunt resistance, and other mechanisms do not induce a significant variation in series resistances. Furthermore, the initial rise of Voc in experimental results could also be explained by a deterioration of electron mobility. This would induce a suplementary reduction of shunt resistance as simulations show on Rsh/Rs plot (right). This analysis shows that a probable cause of degradation of the solar cell investigated by the authors is a deterioration of the perovskite layer. The analysis done here shows a new method to interpret the electrical parameters usually measured during degradation experiments and can be complementary to other characterisation methods in order to understand the complex and various degradation behaviors of perovskite solar cells.

[1] Huang, Y. *et al*. (2021). Limitations and solutions for achieving high-performance perovskite tandem photovoltaics. Nano Energy, 88(2021), 106219.

[2] Khenkin, M. *et al.* (2020). Consensus statement for stability assessment and reporting for perovskite photovoltaics based on ISOS procedures. Nature Energy, 5(1), 35–49.

[3] Lim, J. *et al*. (2021). Kinetics of light-induced degradation in semi-transparent perovskite solar cells. Solar Energy Materials and Solar Cells, 219(September 2020), 110776.