Advanced chemical characterization of Perovskite systems: XPS analysis and depth profiling

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In the past few years, hybrid perovskite solar cells have attracted a considerable amount of research and have undergone rapid development as next generation photovoltaics. It is now established that the interfaces play a fundamental role on the initial performances and stability [1]. Their chemical compositions and structural defects are expected to affect critically the device performances. Thus, we propose here a full XPS study involving surface analysis as well as depth profiling, in order to get further insight into the critical role of interfaces on device behavior.

At first, we dedicated a study to the definition of the optimal procedure to ensure that transfer procedures (from the glove-box to the XPS spectrometer), UHV and X-Ray beam irradiation did not modify the original chemical information. Afterwards, surface XPS analysis and depth profiling were carried out on half cells (triple cation Perovskite / TiO_2 / FTO substrate). The reliability issue of XPS profiling is crucial, especially for this sensitive material but also due to the Ar^+ sputtering itself, known to possibly lead to artefacts among them preferential etching and surface elements redistribution. Using monoatomic bombardment, the reduction of lead (Pb) was clearly highlighted preventing to assess the Pb oxidation degree in depth with such operating conditions. In order to reduce the impact of Ar^+ bombardment damage on perovskite, XPS depth-profiling using cluster Argon ions (Ar_n^+), as an alternative ion source (developed for sensitive materials such as polymers or oxides especially), were also tested on the same stack (Fig. 1). Resulting craters from both sputtering methods were characterized, highlighting a notable difference in morphology for both techniques and opening a reflection on the information collected by XPS on those surfaces.

Finally, in order to probe the modification occurring in the complete device, a coupling between XPS and GD-OES (Glow Discharge Optical Emission Spectroscopy) is envisaged, taking advantage of the two techniques [2]. Specific experimental conditions for both characterizations have to be adapted to match the nature of perovskite materials. This coupling can be a very promising way for a fine characterization of thin films and interfaces, paving the rout to a full understanding of degradation mechanism of perovskite thin layers in order to enhance devices stability and efficiencies.

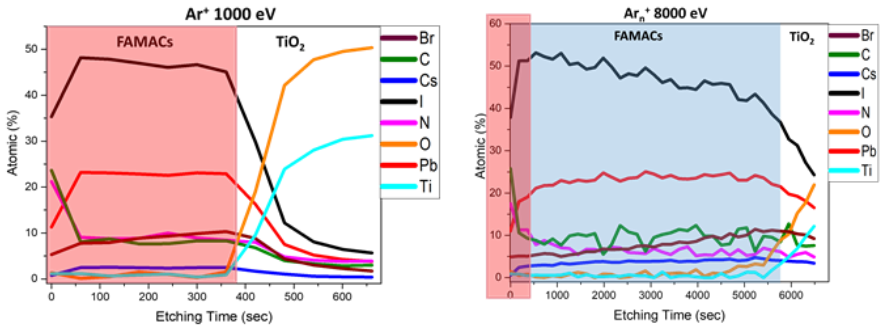

Figure 1. XPS depth profile of FAMACs perovskite layer deposited on FTO / TiO_2 substrate using Ar^+ (left) and Ar_n^+ (right) ion sources

[1] P. Schulz *et al*. Chem. Rev. (2019), 119, 5, 3349-3417

[2] D. Mercier *et al.* Appl. Surf. Sci 347 (2015) 799-807