

In situ Investigation of PbI₂ Precursor Film Formation and Its Subsequent Conversion to Mixed Cation Perovskite

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Abstract : Several deposition methods have been developed for perovskite film preparation. The one-step spin-coating process has emerged as a more popular option thanks to its ability to produce films of different compositions, including mixed cation and mixed halide perovskites, which can stabilize the perovskite phase and produce phases with desired band gap. The two-step method, however, is not understood in great detail. There is a significant need and opportunity to adopt the two-step process toward mixed cation and mixed halide perovskites, but this requires deeper understanding of the two-step conversion process, for instance when using different cations and mixtures thereof, to produce high-quality perovskite films with uniform composition. In this work, we demonstrate using in situ investigations that the conversion of PbI₂ to perovskite is largely dictated by the state of the PbI₂ precursor film in terms of its solvated state. Using time-resolved grazing incidence wide-angle X-Ray scattering (GIWAXS) measurements during spin coating of PbI₂ from a DMF (Dimethylformamide) solution we show the film formation to be a sol-gel process involving three PbI₂-DMF solvate complexes: disordered precursor (P₀), ordered precursor (P₁, P₂) prior to PbI₂ formation at room temperature after 5 minutes. The ordered solvates are highly metastable and eventually disappear, but we show that performing conversion from P₀, P₁, P₂ or PbI₂ can lead to very different conversion behaviors and outcomes. We compare conversion behaviors by using MAI (Methylammonium iodide), FAI (Formamidinium Iodide) and mixtures of these cations, and show that conversion can occur spontaneously and quite rapidly at room temperature without requiring further thermal annealing. We confirm this by demonstrating improvements in the morphology and microstructure of the resulting perovskite films, using techniques such as in situ quartz crystal microbalance with dissipation monitoring, SEM and XRD.

Keywords : in situ GIWAXS, lead iodide, mixed cation, perovskite solar cell, sol-gel process, solvate phase

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