Hybrid Perovskite Solar Cells: *In situ* investigation of solution-processed PbI_2 precursor films used in the two-step fabrication of $CH_3NH_3PbI_3$ films

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Abstract:

Hybrid perovskite solar cells have emerged as a remarkable contender for low-cost fabrication of highly efficient solar cells and modules. Current record efficiency cells with power conversion efficiency exceeding 22% are fabricated using the well-established solution-based two-step method, which consists in deposition of PbI_2 and its subsequent conversion to $CH_3NH_3PbI_3$ by exposing to CH_3NH_3I. This contribution investigates the important step of PbI_2 deposition by spin-coating from a DMF solution. We have used time-resolved grazing incidence wide angle x-ray scattering (GIWAXS) measurements in situ during spin coating, to reveal the formation of a sol-gel process involving three sequential PbI_2·DMF solvate complexes: disordered precursor (P_0), ordered precursors (P_1,P_2) and PbI_2 formation initiated after only 5 minutes in ambient air. The ordered solvates are highly metastable and eventually disappear, leading to formation of the PbI_2 phase at room temperature without requiring thermal annealing. Atomic force microscopy (AFM) and scanning electron microscopy (SEM) were used to further investigate the morphology of the PbI_2 film which has been spin coated and arrested at different phases, then either dried in air or annealed at 100°C. The drying process in addition to the state of the as-cast PbI_2·DMF precursor film at the end of solution processing affect the final morphology of the PbI_2 film. The air-dried PbI_2 film forms substantially more porous films, especially when it is processed from the less ordered P_2 solvate phase, which is desirable for subsequent conversion of the perovskite phase. The study links the PbI_2 thin film morphology to the drying method and reveals its dependence upon the state of the as-cast PbI_2 film from which air-drying occurs. This indicates that the microstructure and morphology of the polycrystalline perovskite films formed by converting PbI_2 may also be affected, with implications for solar cell performance.

Contribution: Oral