MS18-P03 | Phase Evolution During Perovskite Formation - Insight from PDF Analysis

Hua, Xiao (University of Oxford, oxford, GBR)

The recent introduction of organometal halide perovskites to solar cells has significantly enhanced the power conversion efficiency of alternative photovoltaic devices, revolutionizing the development of photovoltaic technologies. To produce perovskite thin films with high device performances, various fabrication methodologies have been developed leading to thin films with different surface structures and crystal morphologies. Tremendous efforts have been devoted to characterizing macro- and microscopic structures within these films to better understand the processing-property-performance relationship. However, their atomic structure and its influence on device performance remains poorly understood. To this end, we employed pair distribution function analysis of X-ray total scattering data to obtain crystallographic and compositional information of methylammonium-lead-iodide ($MAPbI_3$) thin films. This analysis revealed a presence of two near-amorphous intermediate phases with local structures that share subtle but significant correlations with the PbI_2 precursor and the desired perovskite phase. The structure transformation from these intermediates to the perovskite deviates from the intuitive belief where the molecular cations get inserted between the sheets of layered PbI_2 upon the crystallization of perovskite. The knowledge offers critical insight into the perovskite formation pathway and reveals an important link between the short-range structure of the thin films and their corresponding device performance.