Development of perovskite films for photovoltaics via thermal evaporation and hybrid methods

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The advancement of perovskite photovoltaics has been led by solution-based approaches, but there is increasing interest in thermal evaporation methods. These techniques, in addition to being scalable, offer advantages like high uniformity of the layer, low material consumption, conformal substrate coating, and absence of toxic solvents. For co-evaporated methylammonium lead iodide (MAPbI3 or MAPI) solar cells, power conversion efficiencies above 20% have already been demonstrated. However, deposition parameters are not easily transferred to different deposition systems and full reproducibility needs to be demonstrated. A dedicated deposition system is here employed with conic crucibles into low temperature effusion cells, apt for uniform deposition over 10 x 10 cm^2 area. A systematization of the co-evaporation process of MAPI films has been attempted, by monitoring and controlling the growth environment thanks to process data digitalization. First, we separately investigated the evaporation of the precursor materials (PbI_2, MAI) looking at the impact of substrate type and treatment, chamber pressure, crucible filling. Co-evaporated samples were then prepared both with standard depositions and combinatorial approaches. As the evaporation of organic precursors is challenging, a hybrid 2-step method was also explored, consisting of evaporation of the inorganic component plus spin-coating of the organic component. Workflows for accelerated material optimization were introduced based on UV-vis transmittance measurements. The films were then characterized through X-ray diffraction, photoluminescence, SEM, EDS, and spectroscopic ellipsometry. The material was finally tested into n-i-p solar cells with solution processed SnO_2 and Spiro-OMeTAD as electron and hole transport layers, reaching efficiencies around 15%.