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Phase structure engineering approach for obtaining high-quality perovskite films

Bkkar M. (ITMO University), **Olekhnovich R.O.** (ITMO University)
Professor, Doctor of Technical Sciences. Uspenskaya M.V.
(ITMO University)

Abstract:

In this paper, we study phase structure engineering approach as a promising way to obtain high-quality perovskite films, which will lead to an increase in the stability and efficiency of perovskite solar cells.

Introduction:

Perovskite solar cells are considered to be a main alternative to expensive silicon solar cells, due to the combination of high efficiency and low cost [1]. However, instability to environmental ambient conditions impedes their commercialization [2]. Various approaches have been employed to overcome this fundamental challenge in perovskite solar cells, such as phase structure engineering, composition engineering, interfacial engineering, surface-interfacial modification etc., which seek to: enhance the film morphology, reduce the film defects and improve the interfacial processes.

Under the name "phase structure engineering approach" are introduced the following concepts: deposition methods, annealing process, solvent engineering and perovskite-based composite, in order to enhance the perovskite film quality (larger grains size, homogeneous coverage, free-pinholes and lower traps). Deposition methods, including single-step spin coating, two-step spin coating, vacuum-vapor assisted solution and thermal evaporation, affect the perovskite film morphology and defects. In terms of the perovskite film quality, the thermal evaporation is the best method, and the one-step coating deposition is characterized by the lowest cost with simple fabrication. However, the solution deposition method results in the film with many structural defects [3,4,5]. Therefore, further thermal treatment (annealing) is so important to reduce deposition defects and to control morphology of the perovskite film, which its parameters (temperature, annealing medium and annealing time) associated primarily with perovskite components and the deposition method. Generally, temperature (80- 100 °C), annealing in air and a slow gradual process were found to be optimal parameters of annealing process [6,7,8].

Another important method for improving quality of the active layer is solvent engineering, that precisely interferes with the deposition methods and the annealing process, and depends basically on controlling fast nucleation and delaying crystal evolution of the perovskite film (according to Lamer model) by using: *various solvents* (dimethylformamide, dimethyl sulfoxide, etc.), *solvent system* (mixed solvents, mixed solvent-anti-solvent, etc.) and *solvent additives* (water, hydrochloric acid, etc.), where the mechanism of their interaction with perovskite precursors was described by Lewis base-acid adduct approach [9,10,11]. Interestingly, the previous approach (Lewis base-acid) has been used to prepare perovskite-based composite materials, that have attracted significant attention, due to unique improvements in the stability of perovskite solar cells based on them as an active layer. A base is defined as electron pair donor and an acid as electron-pair acceptor, so the perovskite precursors as (CH_3NH_3I and PbI_2) are known to be Lewis acids. Polar aprotic molecules are the most used Lewis bases to form stable intermediate phase (adduct), such as (urea, dimethyl sulfoxide, etc.), but these additives form generally small molecular adducts, so perovskite film with rather spaced grains. Also, Lewis bases, which have lone pair electrons on nitrogen, sulfur or oxygen, as (pyridine, thiophene, etc.), have been used as enhanced material for the perovskite film. However, these types of materials do not hold up harsh environmental conditions because of high molecules volatility and high diffusion coefficients, for this reason, polymeric Lewis bases with a high molecular dipole moment, such as poly (propylene carbonate), have been applied to form inter-grain cross-links and fabricate stable high-efficiency perovskite solar cells. In fact, around the same time, invention about using of (perovskite- polystyrene polymer) composite was announced. Here, also a cross-linked polymer network was formed into perovskite film [12,13,14,15].

Not far from the topic, additives without taking into account the Lewis base-acid adduct approach also were inserted into the perovskite layer, such as (nanofibers, biopolymer (starch), quantum dots), which, in their turn, achieved great results in this field [16,17,18].

Conclusion:

Finally, phase structure engineering is a crucial approach that severely affects the perovskite film quality, thus the overall performance of perovskite solar cells. Depositions method, annealing process and solvent engineering have limited capabilities to control the active film toward the high quality, and their role and effect will end, when the perovskite film takes the final form, but perovskite-based composites have many and varied options to achieve stable high efficiency perovskite solar cells. Specially, perovskite-polymer composite materials play a key compromise role on the way to commercial perovskite solar cells, due to stability improvements that may result from the linking between the perovskite material and the polymer, which leads to larger grain size in perovskite films, reduce traps density, ions migration, charge recombination and improve carrier mobility and life time.