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ХИМИЧЕСКИЕ НАУКИ

WAYS TO INCREASE THE STABILITY OF ORGANIC-INORGANIC PEROVSKITES FOR SOLAR ENERGY

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Introduction. Nowadays, solar energy is becoming an alternative source of energy. The development of technologies for converting renewable energy into electricity is important for the development of society. Perovskite solar cells are a promising new class of solar cells that have aroused great interest and attention of researchers due to their fast growth of power conversion efficiency [1-3]. Organic-inorganic perovskites (OIP) $CH_3NH_3PbI_3$ are relatively easy to synthesize, they have high light absorption coefficients in the visible spectral range and a large diffusion length of charge carriers. However, organic-inorganic perovskites have some disadvantages. They are unstable to moisture, oxygen, UV radiation [4]. The ratio of initial reagents and the chemistry of precursors are the main factors that can affect the structural and, as a result, physicochemical properties of perovskites $CH_3NH_3PbI_3$ [5].

Aim. The aim of this work was to investigate the influence of the ratio of initial reagents on the stability and properties of organic-inorganic perovskites $CH_3NH_3PbI_3$

Materials and methods. Lead iodide (PbI_2) and methylammonium iodide (CH_3NH_3I) were used as initial materials. For the deposition of $CH_3NH_3PbI_3$ films, the initial reagents PbI_2 and CH_3NH_3I with ratios of 1:1; 1:2; 1:3 were dissolved in DMF and stirred at 70 °C for 1 hour. The crystalline $CH_3NH_3PbI_3$ films were formed in a dry box. The previously prepared clear solution was deposited to the purified glass substrate by spin-coating with speed 1200 rpm for 30 seconds. The microstructure of organic-inorganic perovskites was controlled using a scanning electron microscope SEC miniSEM SNE 4500MB. The phase composition of films was identified by X-ray diffractometry (XRD) using a DRON-4-07 diffractometer (Cu*K*α-radiation, 40 kW, 20 mA) over 2Θ = 5–50º, a step of 0.04º and a count time of 4 s.

Results and discussion. The ratio of initial reagents PbI_2 and CH_3NH_3I (1:1; 1:2; 1:3) affects the morphology of the synthesized films. It was established that in the synthesis of films with the ratio PbI_2:CH_3NH_3I = 1:1 the microstructure of the film is represented by anisotropic needle-like particles, with PbI_2:CH_3NH_3I = 1:2 - particles in the form of a maple leaf, and in PbI_2:CH_3NH_3I = 1:3 - particles become more isotropic (**Fig. 1a**). The phase composition of the film depends on the ratio of the initial reagents and the temperature of heat treatment. OIP films $CH_3NH_3PbI_3$ with different ratios of initial reagents are formed according to different schemes: (1) via the formation of three intermediate compounds $(CH_3NH_3)_3(DMF)PbI_5$, $(CH_3NH_3)_2(DMF)_xPbI_4$, $(CH_3NH_3)_2(DMF)_2Pb_3I_8$ (1:1); (2) via the formation of four intermediate compounds $(CH_3NH_3)_2(DMF)_2Pb_2I_6$, $(CH_3NH_3)_2(DMF)_2Pb_3I_8$, $(CH_3NH_3)_3(DMF)PbI_5$, $(CH_3NH_3)_2(DMF)_xPbI_4$ (1:2) and (3) via the formation of two intermediate compounds $(CH_3NH_3)_3(DMF)PbI_5$ and $(CH_3NH_3)_2(DMF)_xPbI_4$ (1:3). In the ratio of initial reagents (1:1) OIP is formed at 115 °C, at a ratio of 1:2 and 1:3 at 170 °C and 175 °C, respectively.

The presence of other compounds in the film can contribute to their stability under the surrounding atmosphere. The influence of moisture on the stability of OIP has been investigated. The stability of perovskite films was determined by X-ray diffractometry and evaluated by the content of the PbI_2 phase, which is formed as a result of the degradation of the OIP film. The X-ray diffractometry results are analyzed and presented as the dependence of the PbI_2 phase content on the time of exposure to moisture (**Fig. 1b**).

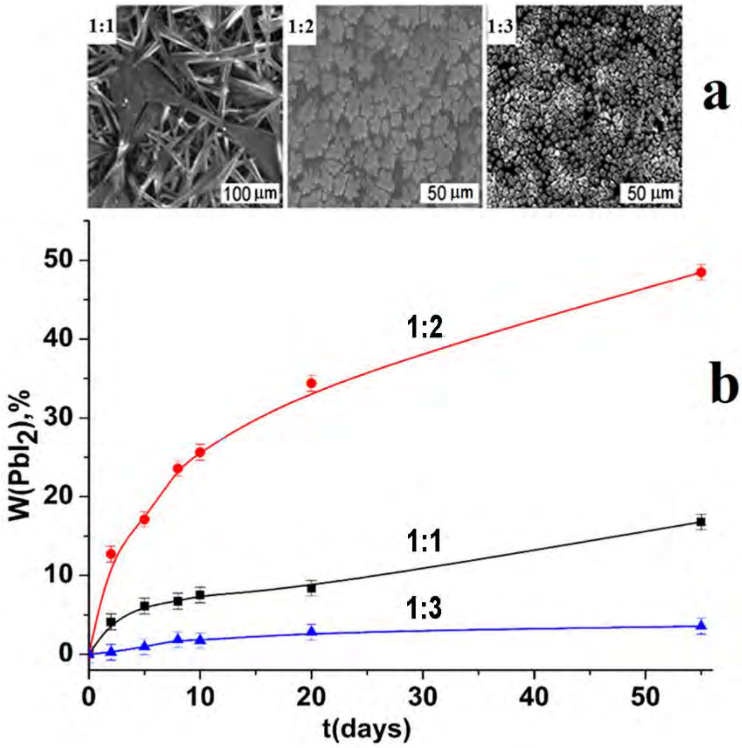

Fig. 1. The microstructure of organic-inorganic perovskite films (a) and dependence of the content of the PbI_2 phase in the decomposition (b) of $CH_3NH_3PbI_3$ perovskite prepared using DMF solvent and different ratios of starting reagents 1:1, 1:2, and 1:3.

It was found that moisture significantly affects the stability of OIP films. Films obtained at a ratio of starting reagents 1:3 are the most stable. The formation of these films of perovskite CH3NH3PbI3 occurs through the formation of 2 intermediate compounds. Films obtained at a ratio of starting reagents 1:2 show the least resistance to moisture, they are characterized by the formation of 4 intermediate compounds.

The formation of perovskite CH3NH3PbI3 at a ratio of 1:1 occurs through the formation of 3 intermediate compounds, and these films show stability to moisture higher than the films obtained at a ratio of starting reagents 1:2, but lower than for films at a ratio of 1:3. Therefore, the presence of a certain number of intermediate compounds affects the properties of organic-inorganic perovskite.

Conclusions. The formation of $CH_3NH_3PbI_3$ perovskite films at different ratios (1:1, 1:2, and 1:3) of the initial reagents PbI_2 and CH_3NH_3I and after heat treatment at different temperatures from 20 to 175 °C were studied. The morphology of the films mainly depends on the ratio of the initial reagents. X-ray diffractometry illustrates that depending on the ratio of the initial reagents and heat treatment temperature of the films, the formation of OIP occurs according to different schemes: through the formation of 3, 4, or 2 intermediate compounds at the ratio of the initial reagents 1:1, 1:2 or 1:3, respectively. The intermediate compounds $(CH_3NH_3)_2(DMF)_xPbI_4$, $(CH_3NH_3)_3(DMF)PbI_5$, $(CH_3NH_3)_2(DMF)_2Pb_2I_6$ and $(CH_3NH_3)_2(DMF)_2Pb_3I_8$ in the films were found. Changing the ratio of starting reagents significantly affects the stability of the films. Films obtained at a ratio of starting reagents 1:3 are the most stable.

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