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Phase Transformations at the Synthesis of Organic-Inorganic Perovskites $CH_3NH_3PbI_3$

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One of the main sources of renewable energy today is solar energy. Among new materials for the efficient conversion of solar energy into electrical are organic-inorganic perovskites, which demonstrate the high efficiency of energy conversion 25.2% [1]. They are an unusual class of materials that combine the advantages of organic and inorganic semiconductors, namely, large optical absorption, high mobility of charge carriers and the variation in the band gap with chemical composition [2]. However, organic-inorganic perovskites are characterized by significant shortcomings that do not allow them to be introduced into mass production today, namely properties degradation over time. Therefore, the cause of this degradation and the means of its prevention is being sought. Today one of the widely used formation methods of thin perovskite films is the deposition of a solution of PbI_2 and CH_3NH_3I compounds in different solvent DMF, DMSO, GBL, NMP onto the substrates. Depending on the solvent nature and the ratio of PbI_2 and CH_3NH_3I, films with different morphology, structural, optical and electrical properties are formed. Our previous investigations have shown that complexes (PbI_3^-, PbI_4^{2-}) are formed as a result of chemical interaction of the organic cation, the coordinating solvent and inorganic components. Such complexes differently affect the properties of perovskites [3]. At the same time, the processes of the formation of intermediates, which can significantly affect the properties of perovskites, are still insufficiently studied. Therefore, the purpose of this work was to investigate the processes of the formation of intermediate compounds at the synthesis of perovskite films $CH_3NH_3PbI_3$ at different ratios of starting reagents, PbI_2 and CH_3NH_3I.

Solutions in DMF of the initial reagents, PbI_2 and CH_3NH_3I in different ratios (1:1, 1:2, 1:3) were used for the synthesis of organic-inorganic perovskites. The formation of perovskite and intermediate compounds was determined by X-ray diffractometry (XRD) and Raman spectroscopy (RS). XRD shows that perovskite $CH_3NH_3PbI_3$ formed by different schemes depending on the ratio of initial reagents: (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 $(MA)_2(DMF)_2Pb_2I_6$, $(CH_3NH_3)_2(DMF)_2Pb_3I_8$, $(CH_3NH_3)_3(DMF)PbI_5$, $(CH_3NH_3)_2(DMF)_xPbI_4$ (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). These results correlate well with RS, which confirmed the formation of the above-mentioned intermediate compounds at certain substrate temperatures. In addition, RS established the presence of DMF solvent molecules in samples in the temperature range from room temperature to 45 °C (for ratio of initial reagents 1:1), to 90 °C (1:2), and to 30 °C (1:3).

[1] National Renewable Energy Laboratory, Best Research-Cell Efficiencies. http://www.nrel.gov/ncpv/images/efficiency_chart.jpg

[2] Saba, M., Quochi, F., Mura, A., & Bongiovanni, G. (2016). Excited state properties of hybrid perovskites. *Accounts of chemical research*, *49*(1), 166-173.

[3] Belous, A., Kobylianska, S., V'yunov, O., Torchyniuk, P., Yukhymchuk, V., & Hreshchuk, O. (2019). Effect of non-stoichiometry of initial reagents on morphological and structural properties of perovskites $CH_3NH_3PbI_3$. *Nanoscale research letters*, *14*(1), 4.