Large-scale fabrication of hybrid perovskites in films by conversion of metallic lead with polyiodide-based reactive inks

Rudnev P.O., Belich N.A., Tarasov A.B.

Laboratory of New Materials for Solar Energetics, Department of Materials Science, Lomonosov Moscow State University, Russia

Hybrid halide perovskites with a general formula ABX_3 ($A=CH_3NH_3^+$, $CH(NH_2)_2^+$, X=Cl, Br, I) are consider to be highly promising materials for the light-absorbing layers of next-generation solar cells. The main synthesis approaches are based on the use of toxic lead salts dissolved in polar aprotic solvents such as DMF, DMSO and GBL that makes them unsuitable for industrially scalable perovskite solar cells production. Thus, new techniques to form perovskite layers with high uniformity are required. It is important also that such new methods should be applicable to form the perovskite layers at a large scale. Earlier the opportunity of one-step conversion of metallic lead into perovskite with reactive polyiodide melts (RPM) AIn (n=3-4) was demonstrated. In theory, such approach allows to obtain large-scale perovskite films. However, there are number of technological difficulties in uniform RPM distribution and control of reaction stoichiometry.

The main purpose of the work is to develop the technique of hybrid halide perovskite films obtained with improved morphology and optoelectronic properties by the conversion of metallic lead with reactive polyiodide melts for scalable perovskite solar cells production. To achieve the goal we need to find conditions for perovskite films synthesis, investigate their microstructural, optical and optoelectronic properties and to fabricate solar cells to prove their power conversion efficiency.

Here, we use spin coating of RPM solution in isopropyl alcohol for uniform deposition of reactive polyiodide melt onto metallic lead surface. The perovskite films are investigated by XRD, SEM, EDX, TRPL, luminescence spectroscopy. Solar cells based on obtained films are fabricated, their IV-characteristics, power conversion efficiency and stability are determined.

We have studied phase formation during the conversion of metallic lead into perovskite with different composition of RPM solution. According to the XRD data, the use of stoichiometric composition MAI_3 does not lead to single-phase perovskite formation without residue of MAI and metallic lead, whereas the use of enriched by I2 (MAI_4) and iodine deficient (MAIx, x<3) composition, with subsequent post-treatment under particular temperature and gaseous environment, allows to obtain single-phase compact films with a thickness of ~500 nm and perovskite crystallites 200-500 nm in size. According to time-resolved photoluminescence data, estimated lifetimes of charge carriers are 45-50 ns. The opportunity of the $MA_xFA_{1-x}I_{3-x}Br_x$ films formation has been demonstrated. Moreover we have fabricated solar cells based on obtained films and measured their IV-characteristics.

Thus, the technique of hybrid halide perovskite films of different composition obtained by the conversion of metallic lead with reactive polyiodide melts has been developed. The solar cells with power conversion efficiency more than 15% have been demonstrated.

The work was supported by Russian Science Foundation (project RSF-19-73-30022).