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Temperature and Moisture Triggered Crystallization of Triple Cation-Mixed Halide Perovskite Cells to Reduce Phase Segregations

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1. Introduction

Perovskite crystallization has not been understood well to date, due to over emphasis on their efficiencies, especially the triple cation-mixed halide compositions. In addition, the difficulty in measuring the critical nucleus sizes in the range of 100 to 1000 atoms shies most experimental method researchers. Synchrotron radiation-based X-ray techniques allow structural characterization providing valuable information about the inner film morphology, e.g., Wide-Angle X-ray Scattering (WAXS) probes length scales in the atomic range and thus yields crystallographic information about the sample[1], while GISAXS is a technique that is surface-sensitive (due to the grazing incidence used) and probes longer length scales, thus providing a full mesoscale approach to the problem of crystallization and the morphology of the samples[2]. The use of fast two-dimensional (2D) detectors with synchrotron radiation allows *in situ* experiments during the growth of perovskites. Sizes, shapes, distances, and correlations of particles are determined from the GISAXS measurements. These parameters will be fundamental in understanding the process of nucleation and growth [3]. In this work, we seek to address the influence of heat stress and moisture probing on the crystallization kinetics of triple cation-mixed halide perovskite cells using in situ WAXS/GISAXS and optical microscopy through photoluminescence.

2. Methods

Cs0.05MA0.75FA0.20Pb(Ix Br1-x)3[4] will be prepared by reaction of CsI, FAI and MAI with an in-organic halide precursor salt PbI2 and PbBr2 . One mole of CsI, MAI & FAI and one mole of PbI2 & PbBr2 in stoichiometric ratios will be dissolved in 1000 µl of dimethylformamide (DMF) and 10 µl dimethyl sulfoxide (DMSO) in ratio of 4:1 for the solvent. The solution will be dissolved overnight at 60° C in a nitrogen filled glovebox. To prepare Cs0.05FA0.75MA0.20)Pb(IxBr1-x)3 films, the 100ul of the precursor solution will be spin coated onto a substrate in two steps of 2000rpm and 1500rpm for 30s. Ethyl-acetate anti-solvent will be introduced after 20s of spin coating to evaporate the solvent from the film. Annealing will be at 1500C for 15 minutes on a hot plate with 500 rpm.

In Situ GIWAXS/GISAXS Experiments:

GIWAXS measurements will be conducted at 23A small- and wide-angle X-ray scattering beamline at the Lawrence Berkeley National Laboratory. The wavelength of X-ray is 1.240 Å (10 keV) and the scattering signals will be collected by a C9728DK area detector. The sample to detector distance will be ≈166 mm, calibrated with a lanthanum hexaboride (LaB6) sample. The incident angle will be kept at 2° to enhance the signal resolution with a frame exposure time of 3 s. The spin-coating process will be conducted in an air-tight chamber under N2 flow, which will consist of a spin-coater and a motorized syringe for remote injection of CB. After the perovskite precursor is dropped on the substrate, concomitant WAXS/SAXS measurement and sample spinning could be triggered simultaneously, followed by a programmed CB injection on the spinning film at a designated timing during the whole 300 s spinning process at 1500 rpm.

In Situ Photoluminescence Microscopy Setup

A Nikon LP-EPILED microscope with a Pixelink PL-B742FF camera will be attached above a bar coating system to observe the kinetics of crystallization of the perovskite solution. Immediately after spreading the perovskite inks, the lens will be lowered in place and the focus will be adjusted to observe the perovskite ink as it dries at the center of the glass substrate. The image stacks will be processed and analyzed by Image J-FIJI to extract the number of crystals, spatial distribution (40× magnification), and area of the crystals (60× magnification)

3. References

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