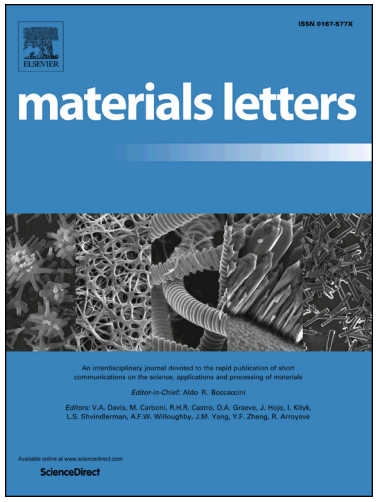

Characterization on crystal structure of $CH_3NH_3PbI_xCl_{3-x}$ perovskite by variable temperature powder X-ray diffraction

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Characterization on crystal structure of $CH_3NH_3PbI_xCl_{3-x}$ perovskite by variable temperature powder X-ray diffraction

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Abstract: In this work the $CH_3NH_3PbI_xCl_{3-x}$ perovskite is obtained by applying vacuum-rotary evaporation procedure with a precursor solution of $PbCl_2$ and CH_3NH_3I in dimethylformamide. Thermal gravimetric and differential thermal analysis (TG–DTA) and the variable temperature powder X-ray diffraction (*in situ* XRD) are employed to research the effect of thermal treatment on the decomposition and the crystal structure of perovskite. It is found that tetragonal to cubic phase transition in the typical perovskite disappears in mixed perovskite crystals because the stabilizing action of Cl. The excess Cl in the precursor leads to the intermediate structure $CH_3NH_3PbCl_3$, and then transforms into $CH_3NH_3PbI_3$ with temperature increasing.

Keywords: Mixed halide perovskite; Thermal stability; In situ XRD; Solar energy materials; Energy storage and conversion

1. Introduction

Since the first report of perovskite solar cells was demonstrated by Miyasaka with power-conversion efficiency (PCE) of 3.8% in 2009 [1], the performance of perovskite solar cells increase at an unprecedented rate. As a light absorber, the PCE of $(NH_2CH_2NH_2)$ PbI_3 perovskite solar cells even get to 22.7% up to now [2]. Because of better device performance, great attentions have been focused on the mixed halide

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