

Supporting Information

Formation of Cubic Perovskite Alloy Containing the Ammonium Cation of 2D perovskite for High Performance Solar Cells with Improved Stability

Mi-Hee Jung^{*,†}

[□]Department of Nanotechnology and Advanced Materials Engineering, Sejong University, 209, Neungdong-ro, Gwangjin-gu, Seoul 05006, Republic of Korea; Fax: +82-2-3408-4342; Tel: +82-2-6935-2597

*To whom correspondence should be addressed.

E-mail: mhjung@sejong.ac.kr

Table S1. Calculated Goldschmidt tolerance factor for alloy perovskites

Compound	r_I/pm	r_{pb}/pm	r_{FA}/pm	r_{MA}/pm	r_{EA}/pm	r_{BA}/pm	t factor
MA _{0.67} FA _{0.33} PbI ₃	220	119	253	217			0.9363
MA _{0.5} FA _{0.5} PbI ₃	220	119	253	217			0.9491
MA _{0.83} EA _{0.17} PbI ₃	220	119		217	274		0.9317
MA _{0.65} FA _{0.3} EA _{0.05} PbI ₃	220	119	253	217	274		0.9400
MA _{0.53} FA _{0.38} EA _{0.09} PbI ₃	220	119	253	217	274		0.9508
MA _{0.65} FA _{0.30} BA _{0.05} PbI ₃	220	119	253	217		517	0.9653

The Goldschmidt tolerance factor, t, defined as follows: $t = (r_A + r_I) / \sqrt{2}(r_{pb} + r_I)$, where r_A , r_{pb} and r_I are the effective radii of cation, Pb²⁺ and I⁻ ions, respectively. The cation radii in mixed-cation materials were calculated based on a weighted average of the radii of cations

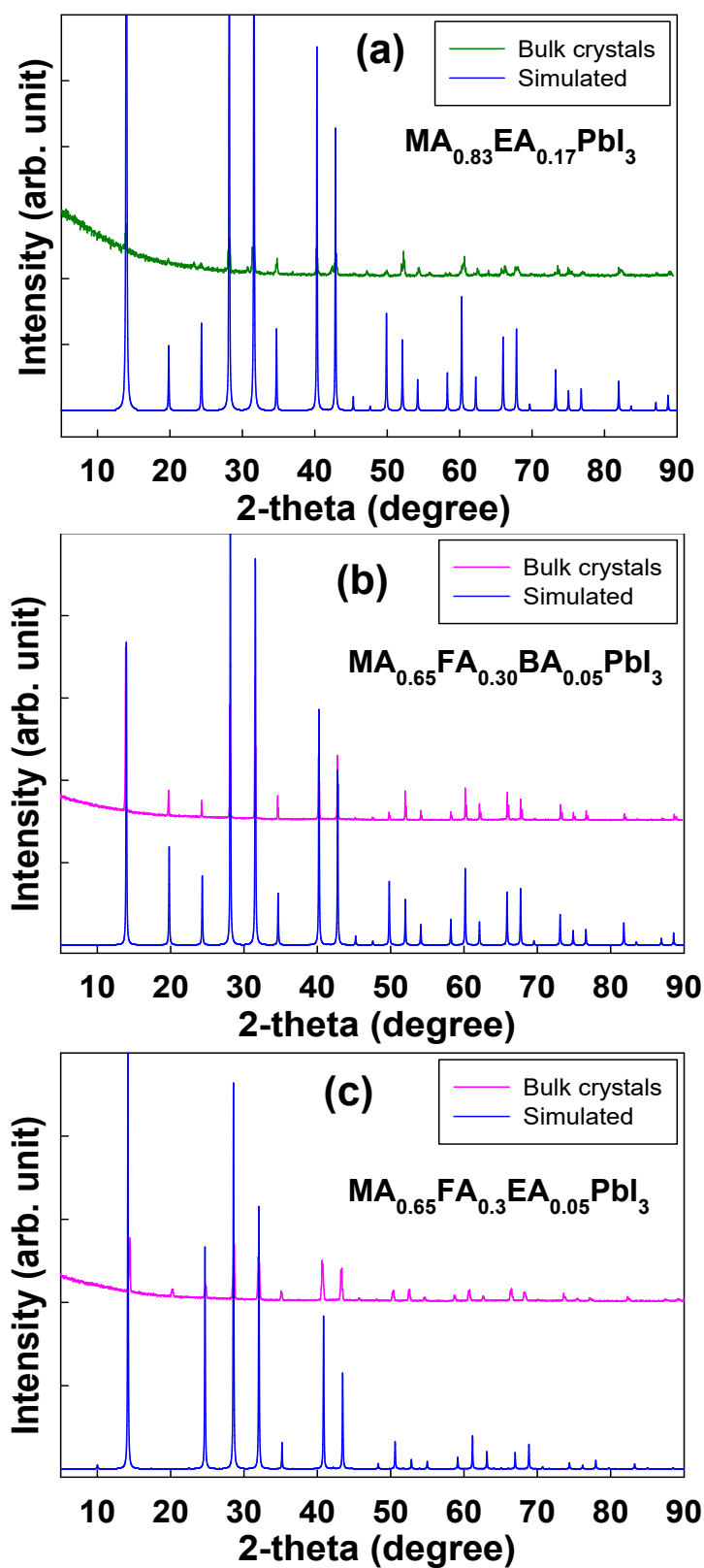


Figure S1. Powder X-ray diffraction and the simulated pattern from SCXRD for the $\text{MA}_{0.83}\text{EA}_{0.17}\text{PbI}_3$, $\text{MA}_{0.65}\text{FA}_{0.30}\text{BA}_{0.05}\text{PbI}_3$ and the $\text{MA}_{0.65}\text{FA}_{0.3}\text{EA}_{0.05}\text{PbI}_3$ perovskites

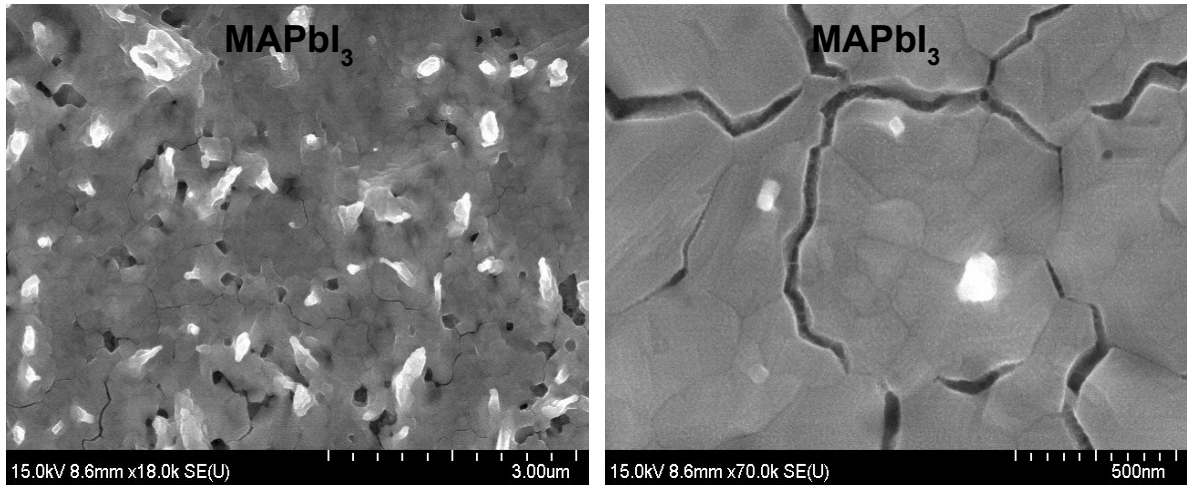


Figure S2. The low and high resolution of SEM images of MAPbI₃ perovskite films.