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Origin of vertical slab orientation in blade-coated layered hybrid perovskite films revealed with in-situ synchrotron X-ray scattering

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Controlling the vertical orientation of perovskite slabs in layered hybrid perovskite films is key for enabling further optimization of photovoltaic device performance. However, the mechanism explaining vertical orientation control in such films remains under debate. Here, we present an in-situ grazing-incidence wide-angle X-ray scattering (GIWAXS) study on the formation of $\text{BA}_2\text{MA}_n\text{-1PbnI}_{3n+1}$ perovskite films during blade-coating where BA, MA and n denote butylammonium, methylammonium and thickness of perovskite slabs. The evolution of grazing-incidence transmission wide-angle X-ray scattering (GTWAXS) signal is also monitored to reveal the specific vertically-oriented low-n phases formed in such films. We find that the blade-coating temperature greatly influences the crystallization dynamics of $\text{BA}_2\text{MA}_n\text{-1PbnI}_{3n+1}$ perovskite films and perovskite slab orientation via intermediate phase and low-n phase formation. For the perovskite film with targeted dimensionality of $n = 4$, blade-coating films at higher temperatures suppresses the formation of the $2\text{MAI } 3\text{PbI}_2 \text{ 2DMF}$ intermediate phase. This in turn suppresses the formation of the $n = 2$ phase that adopts an undesired horizontal perovskite slab orientation, instead favouring the formation of the $n = 3$ phase that adopts the desired vertical perovskite slab orientation. Further analysis on the microstructural evolution of films with near-perfect vertical orientation reveals that the formation mechanism proceeds through several stages: (i) sol-gel, (ii) weakly-texture 3D-like perovskite, (iii) $n = 3$ phase, and finally, (iv) crystallite reorientation into the near-perfect texture. The findings from this in-situ simultaneous GIWAXS and GTWAXS study provide improved understanding of the film formation mechanism for layered hybrid perovskite films with near-perfect vertical orientation.

Presenter Gender

Man

Do you wish to take part in the Student Poster Slam

Condition of submission

Yes

Students Only - Are you interested in AINSE student funding

Level of Expertise

Early Career <5 Years

Pronouns

He/Him

Which facility did you use for your research

Australian Synchrotron

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