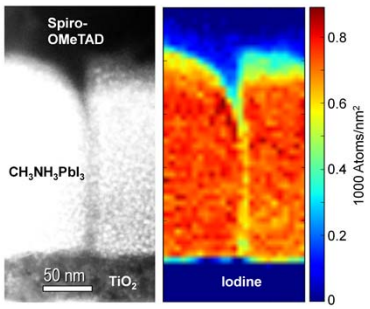
Activating Grain Boundaries in Perovskite Solar Cells



Cross-sectional TEM (left) and compositional analysis by electron energy loss spectroscopy (right) of a hybrid perovskite solar cell. By combining such data with electron beam induced current imaging (not shown), this study reveals how the vertical boundaries between single-crystalline perovskite grains can be activated with hole transport media to efficiently collect photogenerated charges.

This research was performed at the Center for Nanophase Materials Sciences.

Scientific Achievement

A new morphology for perovskite solar cells was realized that activates vertical grain boundaries between single-crystalline grains to enhance the collection and transport of photogenerated charges.

Significance and Impact

This discovery enables an industrially-scalable, cost-effective approach for producing highly-efficient hybrid perovskite solar cells with nearly 100% internal quantum efficiency.

Research Details

- A simple layer-by-layer fabrication process that includes air exposure leads to large single crystalline perovskite grains with vertically oriented grain boundaries.
- The hole-transport medium Spiro-OMeTAD infiltrated into the grain boundaries participates as carrier collector and forms transport channels.
- The prototype cells exhibit an average power conversion efficiency of ~ 16%.

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Narrative Highlight Text:
Organometal halide perovskite films being developed for solar cells tend to form grain boundaries (GBs) during their synthesis, which are know to degrade their efficiency by acting as sinks for photogenerated carriers to recombine. The grains form during solution processing of the lead iodide (PbI_2) and methylammonium iodide (CH_3NH_3I) precursors when large quantities of $CH_3NH_3PbI_3$ seed clusters form. Rather than attempt to grow large area, single-crystal $CH_3NH_3PbI_3$ perovskite films, ORNL researchers discovered how to activate the grain boundaries to harvest nearly 100% of the charges generated by the solar cell. They invented a simple layer-by-layer fabrication process based on air-exposure followed by thermal annealing to grow perovskite films with large, single-crystal grains and vertically-oriented GBs. The GBs were then activated by infiltrating the hole-transport medium Spiro-OMeTAD (2,2′,7,7′-tetrakis[N,N-di(p-methoxyphenylamine)]-9,9-spirobifluorene) to suppress carrier recombination as well as act as active collection channels, resulting in internal quantum efficiencies approaching 100% across the visible spectrum. Prototype solar cells showed an average PCE of 16.3 ± 0.9%, comparable to the best solution-processed perovskite devices. This approach represents a promising path toward theoretical maximum PCE with industrially realistic processing techniques.

Reference

"Perovskite Solar Cells with Near 100% Internal Quantum Efficiency Based on Large Single Crystalline Grains and Vertical Bulk Heterojunctions"
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