

Atomic-scale Defects Critical to the Performance of Perovskite Solar Cells

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Background

Metal halide perovskite semiconductors have emerged as a focal point of research due to their potential applications in solar cells, characterized by exceptional power conversion efficiencies, extended carrier lifetimes, reduced recombination rates, and cost-effective manufacturing techniques. Despite their considerable potential, challenges such as structural instability, ion migration, hysteresis, and defect intolerance are impeding their practical application. There is a critical need for a detailed atomic-scale understanding of the processes that control these properties and performance, however, atomic-scale electron microscopy studies have been relatively limited due to the extreme sensitivity of these materials to the electron beam. Here we develop and apply low dose electron microscopy methods to provide new insights into the structure-property relationships of these materials, including the role of nanoscale heterostructures, octahedral tilts, and point and planar defects, that are critical to their distinctive properties.

Methods

Transmission Electron Microscopy (TEM) offers valuable insights into the local atomic structure of materials. The application of TEM in the study of perovskite solar cells is extremely challenging due to their extreme sensitivity to electron irradiation, which can lead to rapid changes to their pristine structures with doses as little as a few electrons per Å², far below conventional techniques, including STEM, EDX and EELS. To circumvent this limitation, we have developed and applied a suite of specialized TEM protocols encompassing specimen preparation, inert atmosphere transfer, diffraction pattern and image acquisition, and data interpretation.

Results

Our study reveals the sequence of subtle, atomic-level structural transformations leading to the degradation of mixed-cation Cs_{1-x}FaxPbI₃, beginning with the formation and ordering of ion vacancies and followed by a composition-dependent octahedral tilt. Additionally, we elucidate the atomic configurations of planar defects, including twins and Ruddlesden-Popper phases, and establish a correlation between these defects and solar cell performance. Our findings indicate that certain types of twin defects adversely affect solar cell efficiency, and their removal markedly enhances device performance.

Conclusion

The insights gained from our study into ion loss, ion migration, octahedral tilt modes, and the influence of A-cations shed light on the atomic-scale structural mechanisms responsible for the instability of perovskite solar cells. By correlating specific atomic defect structures, including planar defects, with optoelectronic properties, we outline strategies for the amelioration of perovskite solar cells through defect engineering, paving the way for their improved performance and stability.

Keywords:

Low-dose TEM, perovskite solar cells

Reference:

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