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Imaging Buried Dislocations in Halide Perovskites with 3D Strain Mapping

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Halide perovskite have garnered significant attention as materials for use in solar cell and lighting applications, and over the last decade, device efficiencies of halide-perovskite based solar cells have risen from 14.1% (2013)[1] to 25.7% (2022)[2]. However, much of this improvement has been the result of empirical optimisation of fabrication procedures and our understanding of the light absorbing halide perovskite materials lags behind. It has become evident that strain plays an important role in determining device efficiency and long-term stability,[3] but the precise mechanism by which strain affects the materials' optoelectronic properties remains unclear.

In this talk, I will present our recent work investigating the internal structure of the archetypical $MAPbBr_3$ halide perovskite ($MA = CH_3NH_3$) using Bragg coherent diffraction imaging measurements[4] carried out at the Diamond Light Source, UK. This technique allows us to view the atomic displacement fields within our $MAPbBr_3$ material in the form of real space crystal reconstructions. By analysing these displacement fields, we are able to identify $\langle 110 \rangle$ and $\langle 100 \rangle$ edge dislocations in $MAPbBr_3$, the latter for the first time. Further, by using in situ measurements we also uncover that these dislocations become significantly more mobile under illumination with visible light. Solar cells (obviously) must be illuminated during operation, therefore, this light-induced dislocation migration gives us an insight into the buried nanoscale changes occurring in halide perovskite materials during device operation. Further, we intentionally study a subset of crystals that degrade under exposure to the X-ray beam, and by combining the coherent diffraction imaging data with photoluminescence microscopy, we discover that dislocation formation is a key step in material (and therefore device) degradation.

Our results provide unique insight into the nanoscale structure of halide perovskite materials, and show how the internal strain state of the materials evolves with time under operational stressors, and is therefore of significant interest to the halide perovskite, and materials science fields.

[1] Burschka, J. et al. Sequential deposition as a route to high-performance perovskite-sensitized solar cells. Nature, **499**, 316–319 (2013).

Best Research-Cell Efficiency Chart. https://www.nrel.gov/pv/cell-efficiency.html.

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