Ferroelastic Hysteresis in Thin Films of Methylammonium Lead Iodide

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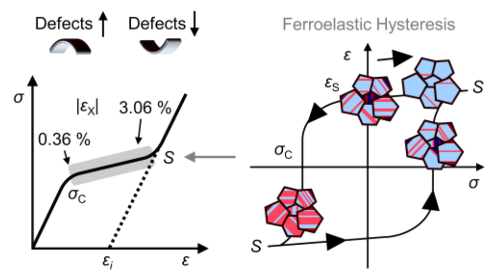
Hybrid halide perovskites of type $APbX_3$ have emerged as materials for solar cells and are attractive for a variety of other thin film devices. However, device performance is hampered by poor material stability and carrier trapping.[1,2] Here, we discuss how ferroelasticity impacts mechanical strain, defects, and degradation in the widely-used methylammonium lead iodide $MAPbI_3$.[3] Specifically, the consequences of ferroelastic hysteresis, which involves the retention of structural memory upon cycles of deformation, are reported for polycrystalline films. Repeatedly bent films were examined using Grazing Incidence Wide-Angle X-ray Scattering (GIWAXS) to quantitatively characterize the strains and proportions of twin domains. Approximate locations for the coercive stress and saturation on the ferroelastic stress-strain curve are identified, and changes to the stress-strain curve with cyclic strain are characterized. Notably, an external stress source, such as thermal stress from the substrate or a roll-to-roll printing setup, must apply at least |50| MPa to modify the proportions of different twins. The presence of specific twin domains is found to correlate with previously-reported strain and defect heterogeneity in $MAPbI_3$ films. Nucleation of new domain walls occurs for specific mechanical strains and correlates closely with degradation. These results help to explain the behavior of ion migration, degradation rate, and photoluminescence in thin films under compressive and tensile strain.



Stress-strain curve of $MAPbI_3$, with the ferroelastic regime and trends in defects and twin populations.

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