Materials Science & Engineering Dissertation Defense

Shedding Light on Atomistic Structures of Defects in Polycrystalline Thin-Film Solar Cells via Simulated X-ray Absorption Spectroscopy

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Abstract

In polycrystalline thin-film cadmium telluride (CdTe) solar cells, the “sprinkle” of dopants and selenium alloy have significantly enhanced hole density and minority carrier lifetime. However, the distribution of their atomic structures is still unclear.

Herein, X-ray absorption near edge structure (XANES) was used to probe atomistic structures of dopants and defects in CdTe. This work built a bridge between theory and experiment by performing simulations of XANES spectra from predicted defect models – mostly from density functional theory (DFT) and some by educated guess. Then, by linear fitting, the simulated spectra were used to extract atomistic structures from experimental spectra of the solar cell devices

XANES analysis of various device architectures reveals structural inhomogeneities across the absorbers from point defects in bulk to secondary phases. The majority of the dopant atoms either 1) do not enter the target lattice sites (they formed secondary phases) or 2) they do enter the target site but form complexes with impurities, resulting in low dopant activation and compensated hole density. In operando, XANES analysis revealed the atomic reconfiguration around the dopant atoms and their possibly altered electronic structures.

Complementary to the DFT prediction, this work provided the distribution of selenium local structures across the absorber, specifically the variation of Se-Cd bond lengths in different performing areas. Under environmental stressors (heat and light), it showed selenium diffusion into the bulk, co-occurring with device degradation.

This framework was also extended to study defect evolution in other thin-film solar cells (CIGS and emerging perovskite). XANES analysis has shed light on atomic defects governing solar cell performance and stability, which are crucial in pushing the efficiency toward the theoretical efficiency limit.

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Zoom Link:

https://asu.zoom.us/j/82706472079?pwd=MHEwNVJZY21QeGs2RkpmR2dUUXMydz09

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