Operando X-ray Diffraction of $CH_3NH_3PbI_3$ Solar Cells

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ABSTRACT

Methylammonium Lead Iodide ($CH_3NH_3PbI_3$) organic-inorganic perovskite films are a promising absorber material with solar cell efficiencies now in excess of 21%. A significant appeal of these materials is their facile synthesis using solution processes. Typically a low temperature anneal (about 100 °C) is involved in film synthesis with subsequent cooling through the cubic-to-tetragonal phase transition near 65 °C. Since the transition temperature is within the range expected in real world device applications, it is therefore important to understand the structural behavior at this transition and its impact on the device performance. In order to better understand this phase transition in thin films, we have developed the capability for *operando* synchrotron X-ray diffraction by designing a sample stage for simultaneous, temperature dependent measurement of J-V curves and diffraction. This has allowed us to obtain X-ray diffraction data during the operation of $CH_3NH_3PbI_3$ devices. Here we will present structural characterization of the perovskite crystal structure with increasing temperature. The impact of these structural changes on the device J-V characteristics will be described and we comment on potential implications for material and device properties.

ABOUT THE SPEAKER

Laura T. Schelhas is a postdoctoral scholar in the Materials Science Division at the Stanford Synchrotron Radiation Lightsource (SSRL) at SLAC National Accelerator Laboratory. Her research mainly focuses on understanding the structure function relationship in optoelectronic materials for application in photovoltaics (solar panels). This work utilizes in-situ and operando X-ray diffraction techniques to look at both the formation of materials as well as degradation mechanisms in operational cells. She also works closely with theorists to inform materials by design creating a feedback loop between theory and experiment. She received her Ph.D in chemistry from the University of California, Los Angeles (UCLA) in 2013 where she studied the influence of nanoscale architecture on the materials properties in magnetic and magnetoelectric materials, performing high resolution X-ray diffraction experiments at SSRL during her studies. In 2014, she accepted her current position at SSRL.