Determining bandgap profiles and sub-gap defect levels in solar cells using high resolution electron energy-loss spectroscopy

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Information on bandgaps, defect states, and other electronic transitions, is essential for understanding functionality and degradation of semiconductor materials. While high-resolution imaging using aberration-corrected scanning transmission electron microscopy (STEM) provides a path for elucidating structure in the vicinity of defects and interfaces, it provides little insight into the electronic properties. Recent improvements in energy resolution, as a result of advances in electronics, optics and monochromation, open up the opportunity to obtain such information using electron energy-loss spectroscopy (EELS). In this contribution, we will present results from our research on the use of low-loss EELS for investigation of two important topics in $CuIn_{1-x}Ga_xSe_2$ (CIGS) solar cells: spatially-resolved bandgap profiling and detection of sub-gap defect states. The research was carried using a monochromated FEI Titan[3] G2 STEM operating at 60 kV and with an energy resolution of 130 meV.

For the first topic, we will discuss a new, simplified bandgap extraction method, based on a straightforward Gaussian fit model, that was developed to enable more rapid and robust bandgap profiling. The applicability of this technique will be demonstrated via bandgap profiling through a CIGS solar cell containing intentional Ga/(Ga+In) compositional gradients, and thus bandgap gradients. Comparison of the EELS-based bandgap profile to the nominal profile calculated using STEM-based energy dispersive X-ray spectroscopic composition data shows excellent spatially-resolved agreement. While this approach sacrifices a small degree of absolute (systematic) accuracy, excellent internal precision is maintained, and the effectively intervention-free methodology improves analytical speed and robustness.

Spatially resolved characterization of electrically active defects with energy levels within the bandgap is a significant challenge in CIGS (and in many semiconductor materials). Such defects can limit/prevent achievement of maximum device performance. The challenge is to be able to correlate these defect energy levels with specific structural defects. To this end, we will present recent work on the energy- and spatially-resolved detection of sub-gap defect levels (carrier traps) within two different CIGS samples with two different trap energies (E_V + 0.43 eV and E_V + 0.56 eV). Low-loss EELS is shown to not only enable spatially-resolved detection of these states, but is also found to provide identical energies as those obtained using conventional and accurate deep level transient spectroscopy (DLTS). Furthermore, correlation between a new scanned probe DLTS method and low-loss EELS show accurate correlation in both spatial localization and sub-gap energy position.

These results demonstrate the potential of high-resolution EELS for the spatially resolved characterization of important electronic structure details in semiconducting materials, and illustrate how correlation with other characterization techniques can be used to yield new insights into structure-property relationships in complex functional materials.