BAPVC Annual Project Report
Project Title: Advanced Materials Characterization
PI: Mike Toney & Alberto Salleo
E-mail: mftoney@slac.stanford.edu, asalleo@stanford.edu

Summary:
The Toney Group at SSRL characterizes photovoltaic materials with X-ray techniques. A method of determining whether CZTSe is in the kesterite and stannite phase utilizing resonant diffraction has been developed and CZTSe films (NREL, Utah, DuPont (future)) have been characterized to determine the phase distribution and level of homogeneity and correlate these properties with their PV performance. The work of the Salleo group within BAPVC focuses on using sensitive sub-gap measurements to characterize optical absorption and defects in photovoltaic materials and entire PV stacks.

Key Accomplishments:

The kesterite and stannite phase are indistinguishable by standard XRD measurements because the two phases are distinguished by the placement of the zinc and copper atoms within the lattice structure. The distinction between these two phases is important, as their PV properties are dramatically different. Modeling has been done to show that using resonant diffraction the ordering of the copper and zinc atoms can be distinguished (Figure 1). This modeling has been verified to be able to distinguish between the two phases of CZTSe in measurements done at SSRL.

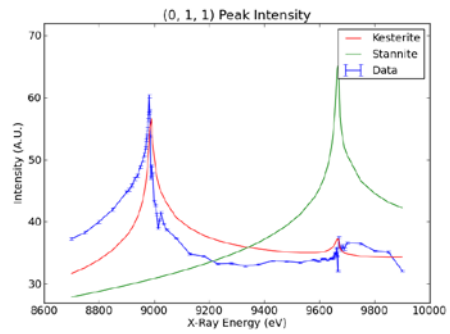

Figure 1: CZTSe resonant diffraction data (blue), model of stannite resonant diffraction (green), model of kesterite resonant diffraction (red).

By combining the Transmission X-ray Microscope (30 nm resolution) ability to probe a material with element specificity and ability to image this information in a 2-D or 3-D manor it is possible to understand the distribution of the component elements with in a material and to extract out from this the distribution of the materials. This technique has been demonstrated (Figure 2) and in this case the lack of homogeneity may explain the samples poor performance.

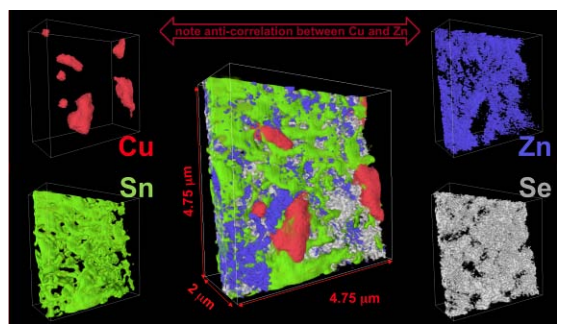

Figure 2: TXM tomography image of a CZTSe sample delineated by element with copper shown in red, tin shown in green, zinc shown in blue and selenium shown in gray.

True absorption (i.e. excluding scattering) above gap was done using photothermal deflection spectroscopy (PDS) in thin and thick layers. PDS was used to measure the absorption of a thin (320 nm) unpatterned Si membrane and compare it to the patterned Si membrane produced by the Atwater group. The results demonstrate that the pattern designed produces a 200X broadband enhancement, well above the Yablonovitch limit (~50X).

The Scarpulla group is developing a laser-based technique to anneal CdTe defects using high-power Nd:YAG radiation. Using PDS the sub-gap of CdTe films laser-annealed in

different conditions has been characterize. Compared to the unannealed reference signal, a reduction in subgap absorption around 1.2 eV was observed in all the annealed films. These preliminary results however were inconclusive due to a strong absorption between 0.5 and 1 eV probably due to the FTO underlayer. The experiments will be repeated without the FTO layer.

3Sun operates an a-Si:H/micromorph tandem facility and is testing different deposition conditions for the a-Si:H. Measurements of a-Si:H cells with different thicknesses and recipes were done using FTPS to determine whether the increase in hydrogen content affects the amounts and distribution of sub-gap defects in the stack. Looking at the data in a semi-log scale reveals that the sub-gap signal does not depend on the hydrogen content (Figure 3).

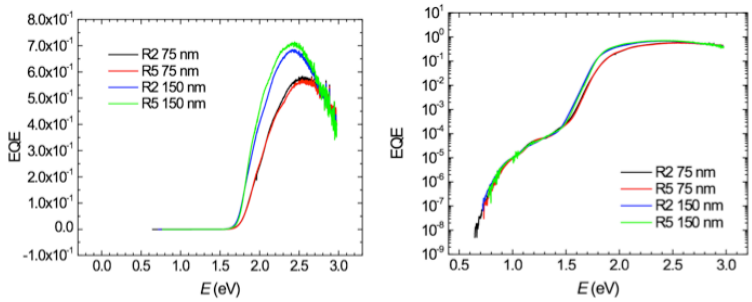

Figure 3: EQE of 4 3SUN cells showing that thicker cells generate more current (left). Sub-bandgap EQE of all cells showing that the shape of the defect DOS is independent of hydrogen content in the plasma (right).

Future Work:

The resonant diffraction work described here for CZTSe has been demonstrated to work and moving forward the goal is for additional members of the Bay Area Photovoltaic Consortium to be able to utilize these techniques on CZTSe films. It is also believed that both other BAPVC members with CZTS and other materials could benefit from TXM characterization and moving forward this will be demonstrated. This will include the silver silicon interface of DuPont's silver paste with the solar cell. CIGSe will also benefit form this technique. Work is also being done to developed in-situ diffraction annealing chambers capable of supporting a selenium rich environment for materials such as CZTSe and CIGSe. Future work will be done on 3Sun a-Si:H cells to discover the origin of the sub-gap states.