BAPVC Annual Project Report

Project Title: In Situ Characterization of Grain Growth in Thin Film Semiconductors
PI: Delia Milliron
E-mail: dmilliron@lbl.gov

Summary:
Thin film absorbers are prepared from solution processed nanocrystals of the same composition, including CZTS, CIGS, and CIS. A thermally-induced metastable-to-stable crystal phase transition is leveraged as a driving force for grain growth and surface chemistry is under development that can supplant conventional selenization processes. Materials evolution during processing is followed by x-ray diffraction, Raman, and SEM and the resulting microstructures are now being correlated with electrical properties of the materials.

Key Accomplishments:
The work undertaken during the past year involved the successful development of solution syntheses of CZTS, CIGS and CIS nanocrystals with tight control over their composition, shape, and crystal structure. These nanocrystals have been used to study grain growth through thermal treatment routes, applying both *in-situ* and *ex-situ* methods (Figure 1). Both *in-situ* and *ex-situ* studies show that thin films of absorber materials with average grain sizes up to one micron can be accessed from few-nanometer size crystallites without the need of traditional high temperature selenization process. Significant time was spent in order to optimize the annealing procedure. This required cross section SEM analysis with simultaneous x-ray diffraction and Raman analysis. These results represent the first report of grain growth without selenization from these compound semiconductor nanocrystals. Also a new insights into the role of surface chemistry in influencing grain growth has been gained by surface functionalization of these nanocrystal with chalcogenidometallate clusters (ChAMs) and the impact of this functionalization on the grain size and electronic properties has been also started.

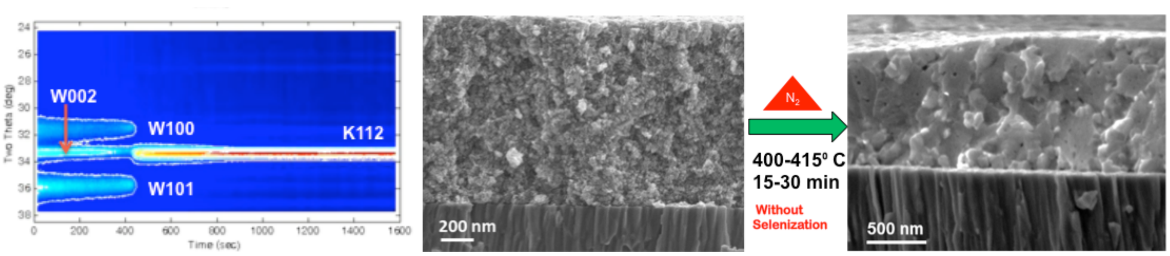

Figure 1: (a) Real-time analysis (*in-situ*) of phase transition and grain growth of compound semiconductor nanocrystals by XRD. (b) & (c) SEM images shows the micron thick nanocrystal film obtained through drop-casted method on Mo-coated substrate and subsequent thin film formation with micron size grain achieved after annealing at low temperature.

Future Work:
The future work will be focused in optimization of the grain growth process over device scale areas with controllable thickness and grains to form good absorber layers, which will be further used to fabricate full PV devices. Hall measurements will be correlated with microstructure and applied to interpret the characteristics of the PV cells. Systematic studies will be carried out to correlate the metastable-to-stable phase transition of the nanocrystals and it’s relationship to grain growth, all as a function of the surface (ligand) chemistry. We will continue to employ in situ x-ray diffraction, ex situ SEM analysis, and Raman spectroscopy to follow to course of these transformations.