Project 05: Project Progress Summary – Fall 2012 to Fall 2015

Nanowires of copper, indium, gallium and selenide (CIGS) and copper, indium and selenide (CIS) have been synthesized by two separate processes: one by chemical vapour deposition (CVD) using the vapour-liquid-solid (VLS) mechanism, the other following an hydrothermal method. Growth by CVD is sensitive to a number of parameters including carrier gas flowrate, the temperatures of the source materials, the temperature of the growth substrate and the nature of the catalytic film employed to assist with deposition. A systematic study has been performed in order to establish the optimum range of conditions for CVD for these materials. Scanning electron microscope (SEM) imaging of samples show that, under the appropriate conditions, nanowires are formed, while energy dispersive spectroscopy (EDS) reveals the composition of the structures. Photoluminescence measurements have been performed on samples in order to characterize their optical properties.

A parallel fabrication process, adopting an hydrothermal-based approach, has been pursued in developing heterostructures of zinc oxide (ZnO) and CIS. Such heterostructures, consisting of a ZnO core and CIS shell, have been grown. SEM images show that nanotubes of ZnO may, under the right process conditions, be generated, while EDS and X-ray diffraction (XRD) measurements confirms that the composition of the heterostructures is indeed ZnO and CIS. Indeed, XRD also shows that variation of certain process conditions - temperature and immersion time - the relative proportions of copper and indium in the CIS material may be controlled. Analysis of transmittance measurements of heterostructure samples containing differing ratios of copper and indium show that a red shift in the band gap of CIS occurs with increasing indium concentration.

Computational calculations of the bandgap of CIS and copper gallium selenide (CGS) have been performed using density functional theory (DFT), using a variety of different functions. Extended Hückel Theory (EHT) calculations, where the density of states for different compositions of $CI_xG1\text{-}xS$, have also been performed.