Project 05: Copper Indium Gallium Selenide (CIGS) Nanowires for Photovoltaic Applications

Project Leader: Harry E. Ruda (HR) - *Centre for Nanotechnology, University of Toronto*
Project Co-applicants: Alain Rochefort (AR) – *École Polytechnique, Montréal*
Project Supporting Partner: Prised Solar

Overview

In the continued development of low cost, high efficiency solar cells, those based on copper (Cu)-indium (In)-gallium (Ga)-selenide (Se) (CIGS) thin films offer an attractive solution due to their relatively high efficiency (~20%) [1] and large optical absorption coefficient (> 10^4 cm^{-1}) [2]. Furthermore, the direct band gap may be tuned (~1-1.7 eV) through control of the amount of Ga impurity present in the CIGS thin film [3]. The large efficiency observed with CIGS thin films is partly ascribed to the formation of nanoscale *p*-*n* junctions comprising of Cu-rich (*p*-type) and Cu-poor (*n*-type) domains randomly distributed within individual grains of a polycrystalline film [4], providing separate physical pathways for electron and hole movement, thus reducing recombination. However, efficiency may be further improved by turning to nanoscale structures, and in particular nanowires, upon which to base next-generation solar cell devices [5,6].

The attractiveness of fabricating nanowire structured photo-absorbers is the potential of obtaining higher absorption due to (i) a concentration in the density of states spectrum in thin nanowires, (ii) an enhancement in local field due to dielectric constant, (iii) long minority carrier lifetimes and carrier diffusion lengths owing to their single crystal format and due to phase space filling, particularly for narrow nanowires, and (iv) enhanced light trapping in appropriately designed nanowire structures. Moreover, a number of recent papers have shown that the complexity of clustering and ordering in multi-component alloys in nanowires reflect inhomogeneous strain distributions, differential migration of species in such structures as well as of formation energies for different phases in such nanostructures [7,8]. Hence, the optimum composition and temperatures for formation of such structures are far from clear.

We propose to study the conditions for preparation of CIGS nanowires having different alloy composition and dimensions, including core-shell structures. As discussed above, the direct band gap of the material may be tuned, through control of the concentration of the Ga impurity, such that it may be aligned with the optimum band gap for a solar cell absorber (1.1-1.3 eV) [9]. Additionally, the ratio of copper (Cu) to indium (In) in the semiconductor is key to defining its character: Cu-rich structures yield p-type semiconductors [10,11,12]. Thus, the role of material fluxes and growth temperature on compositional, as well as structural, homogeneity are to be examined, through high resolution TEM (HR-TEM) studies. Drawing upon our extensive experience in the preparation of compound semiconductor nanowires [13,14,15,16], we adopt a chemical vapour deposition (CVD) technique employing the vapour-liquid-solid (VLS) mechanism of growth to realise CIGS nanowires. Compositional/structural homogeneity is to be correlated with optical and transport properties measurements on single nanowires by steady state and dynamic photocurrent and photovoltage spectroscopy. In conjunction with empirical investigations, Tight Binding (TB) calculations are planned, in order to study the influence of composition and dimensions of homogeneous and core-shell CIGS nanowires on their overall electronic properties, and to investigate the effect of clustering and ordering within such structures. In addition, Density Functional Theory (DFT) and TB will be employed to understand structural and chemical defects in the vicinity of core-shell interfaces. The associated band-gap and density of states distribution will be extracted from both DFT and TB electronic structure calculations.

Based on our previous work on preparing high quality electro-deposited ZnO:Al (AZO) films [17], we will study the conditions required to infiltrate p-CIGS nanowires with n-AZO and characterize the optical and electrical characteristics of such hetero-junctions. In particular, an important objective is to establish the role of interfacial recombination, and charge separation and transport using temperature dependent measurements. We will consider various approaches to ameliorating these effects including interfacial buffer layers and annealing/passivation methodologies.

The principal objective of the study will be to understand how to design CIGS nanowire-AZO-based hetero-junctions suitable for consideration for next-generation solar cells.

References

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