Scanning Transmission Electron Microscopy investigations of an efficiency enhanced annealed $Cu(In_{1-x}Ga_x)Se_2$ solar cell with sputtered Zn(O,S) buffer layer.

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Abstract

$Cu(In_{1-x}Ga_x)Se_2$ (CIGS) is a direct band gap semiconductor widely used in energy conversion devices due to the high sunlight absorbance and high temperature stability. A conventional CIGS solar cell is presented as a stack of glass/Mo/CIGS/CdS/i-ZnO/ZnO:Al. The highest efficiencies are typically obtained with a CdS buffer layer deposited by chemical bath deposition (CBD). However, at the industrial scale CBD generates a toxic waste since Cd is a carcinogenic material. Therefore, a transition to Cd-free buffer layers deposited by a dry vacuum process is mandatory for low-cost and environmentally friendly CIGS photovoltaic in-line production. Thus, sputtered $ZnO_{1-x}S_x$ ($ZnO_{0.75}S_{0.25}$) appears to be an alternative to the CBD CdS buffer layer in CIGS solar cells, providing a negative conduction band offset [1]. Many studies have been conducted in this direction and have shown very promising results [2]. Recently, a significant efficiency enhancement has been reported after an annealing treatment of the complete solar cell stack with the sputtered buffer $ZnO_{0.75}S_{0.25}$ [3]. This enhancement was attributed to an inter-diffusion occurring at the absorber/buffer layer interface. In this work, we investigate by advanced scanning transmission electron microscopy (STEM) techniques, the interface of a similar CIGS solar cell before and after 200°C annealing. In fact, our high resolution STEM (HR-STEM) and energy dispersive X-ray spectroscopy (EDX) demonstrate the absence of any inter-diffusion or intermixing layer at the absorber/buffer layer interface. Interestingly, we systematically observe the presence of stacking faults in close proximity to the absorber/buffer layer interface, independently from the annealing process. Finally, we demonstrate by HR-STEM imaging an order occurring between some $ZnO_{0.75}S_{0.25}$ crystals and the CIGS absorber crystals where an epitaxial relationship is observed between the $ZnO_{0.75}S_{0.25}$ and the CIGS planes subsequent to the 200°C annealing. This change at the CIGS/buffer interface could result in a lower density of interface defects, which in turn would explain the efficiency enhancement observed in the heated solar cell stack.

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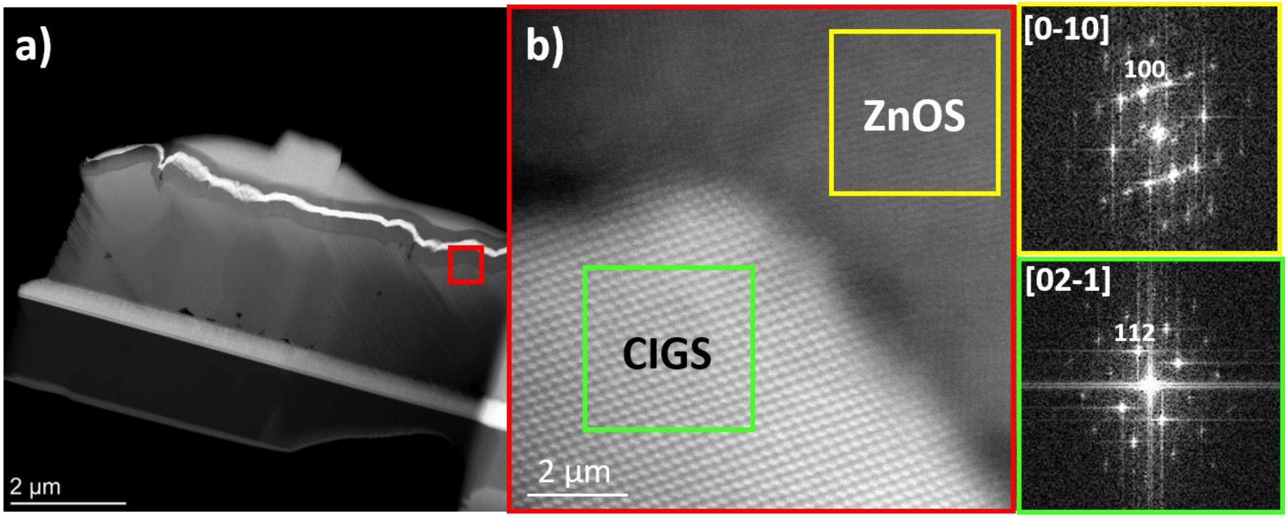

Figure 1: a) STEM-HAADF image of a FIB lamella extracted from the annealed sample. b) High resolution STEM-HAADF image of the Zn(O,S)/CIGS interface with the corresponding Fast Fourier Transform (FFT).