

Efficiency improvement of Cu₂ZnSnS₄ solar cell by optimizing the interface chemistry

Kaiwen Sun, Chang Yan, Jialiang Huang, Heng Sun, Aobo Pu, Martin Green, Xiaojing Hao*

School of Photovoltaic and Renewable Energy Engineering, University of New South Wales (UNSW), Sydney, NSW 2052, Australia E-mail: kaiwen.sun@unsw.edu.au

High bandgap kesterite Cu_2ZnSnS_4 (CZTS) has attracted world-wide attention in recent years owing to the earth-abundance and non-toxicity of its constituents and the realization of high and stable performance [1]. The large deployment of photovoltaic (PV) in the future would demand stable, abundant and non-toxic materials similar to Si, in either flexible/rigid single junction thin film solar cells or tandem cells with Si bottom cell. In this regards, CZTS is more advantageous over other single junction cells and their associated top cell for tandem cells. For its industrial-scale deployment, obtaining high efficiency CZTS is the first prerequisite. Until recently, however, state-of-the-art CZTS devices were limited under 10%, being far below the Schockley-Queisser (SQ) limit of about 33% efficiency under terrestrial conditions [2]. Major limitations lie in the large open circuit voltage deficit (Voc-deficit) and a comparably low fill factor (FF). The loss mechanisms for the Voc and FF have been extensively investigated and the hetero-junction interface quality is one the most proposed factors that contribute to the performance limit.

One of the critical elements of forming a desirable interface structure in hetero-junction PV technology is the junction-formation step [3]. At present, the preferred approach in CZTS community is to deposit a thin CdS layer by chemical bath deposition (CBD) method, where a suitable amount of ammonium hydroxide (ammonia) is applied as the complexing agent. The function of the ammonia has been extensively studied in CIGS (1) clean the absorber surface before the deposition, (2) control the cation slow release, (3) supress the formation of detrimental impurity like Zn(OH)2 at the interface and (4) minimize the metastability behaviour of the device. In our successive ionic layer adsorption and reaction (SILAR) process for alternative ZnCdS buffer deposition, however, no ammonia has been applied. In order to further optimize the interface quality, we explored adding ammonia in the cation solution to realize its similar function in CdS deposition process.

In summary, the CZTS/ZnCdS interface quality is optimized by applying ammonia as complexing agent in the precursor solution during the SILAR process for ZnCdS deposition. Excess oxide and hydroxide impurities formed at the interface are limited to a low level, which reduces the related electronic defects in the depletion region and alleviates the metastability behavior caused by the Zn(OH)₂. The application of ammonia also enables the control of reaction mechanism, improving the epitaxial growth, thereby reducing the interface recombination. Finally, efficiency of up to 10% is achieved by modifying the interface structure thanks to the chemistry method.



Figure 1. X-ray photoelectron spectra (XPS) of O 1s in the ZnCdS film deposited on glass substrates with low (a) and high (b) ammonia concentration. The XPS measurement was performed immediately after 30s etching the surface of each ZnCdS film.



Figure 2. a) Current density-voltage (J-V), b) external quantum efficiency (EQE) curves of devices applying ZnCdS buffer deposited with low and high concentration of ammonia