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Effect of the absorber layer band-gap on CIGS solar cell

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ABSTRACT

The efficiency of Copper Indium Gallium Diselenide solar cell has been steadily increasing over this last decade to reach a record value of 21.7% by the year 2014 complemented with a noticeable cost reduction. The observed improvement in performance could be attributed to the advance in growth and production techniques bringing forth best quality CIGS thin-films. The most attractive property of CIGS compound is the ability to tune its energy band gap from 1.01 eV up to 1.68 eV by variation of Ga fraction leading to a best match to the solar spectrum. In the present work we demonstrate the improvement to be gained if the CIGS band gap is optimized. First, the energy band gap of CIGS absorber layer was varied uniformly to find the optimal Ga content. The simulation is carried out using the solar cell simulator SCAPS-1D. It is found that maximum efficiency of about 22.95% can be achieved with a band gap of around 1.48 eV. In the second set of investigations, a graded band gap absorber is examined. In this simulation several configurations were examined the maximum efficiency obtained is 24.34%.

1. Introduction

Cu(In,Ga)Se_2 (CIGS) is being seen as one of the most promising thin-film solar cell technologies with highest confirmed efficiencies. The most recent record efficiency obtained in a laboratory environment is 21.7% [1,2]. It is common practice, in traditional thin film solar cells, to optimize the absorber material band gap energy E_g: this is the well known trade-off between high current for low E_g and high voltage for high E_g. Present day, high performance thin film CIGS solar cells however use more sophisticated band gap profiles, almost always involving a grading of the band gap E_g throughout the absorber layer, consequently a changing of most material properties across the cell. This is achieved by introducing a spatial variation of Ga and/or S content within CIGS layer. Poor electronic properties of wider band-gap CIGS absorber layer leads to a low fill factor and a high recombination rate, this kept the optimum E_g not further than 1.3 eV [3]. With the introduction of new production techniques, such as the alkali post deposition treatment (PDT) [1], control of lattice-induced defects becomes possible, thus enhancing CIGS electronic quality. Improvement of wider band-gap CIGS has also been reported for devices grown with higher than standard substrate temperatures [4]. Therefore, high efficiency of uniform band-gap CIGS solar cells with E_g matched to the theoretical optimum Shockley- Queisser conversion efficiency could be achieved.

A non-uniform Ga/(Ga+In) ratio throughout the absorber layer, commonly termed as Ga-grading, allows the creation of an in-depth band gap variation, so an additional electric fields into *p*-type CIGS absorber. This band gap profiling is often classified in two types, single and double grading. Single grading is an increase of the band gap towards the back or towards

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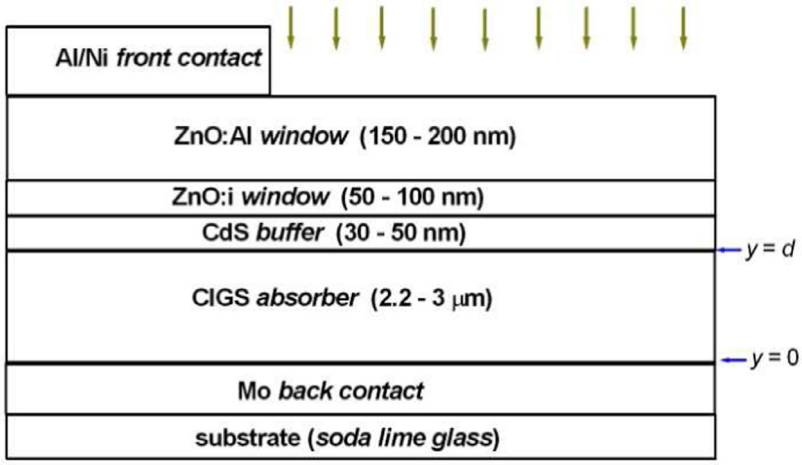

Fig. 1. Schematic diagram of a ZnO/CdS/CIGS solar cell, only semiconductor layers are reproduced in numerical models. The metallic contacts at the top and bottom are defined by their work functions and surface recombination velocities.

the front contacts, while the double grading profile has a minimum band gap some distance into the CIGS layer and an increased band gap both towards the back and front contact [5]. It has been proven that this band-gap gradient enhances significantly the performance of CIGS solar cells. Several numerical modelling tools, like AMPS and SCAPS, are used to show that there can be a beneficial effect of grading [6–9]. The underlying idea is that it should be possible to increase the cell efficiency by realizing an optimized band gap profile.

In this paper two different approaches are explored, the first consists of varying Ga content uniformly throughout the CIGS absorber layer to investigate the effect of increasing E_g on cell performance, including wide band-gaps. The effect of higher uniformly varying energy band-gap has not been thoroughly analysed because it has been reported in literature that the device performance degraded when E_g exceeded 1.3 eV [10,11]. In the second approach a graded CIGS absorber is analysed by assuming a spatially linear variation of the Ga ratio. To examine all possible cases the band-gap values at the front and the back of the CIGS layer are changed independently, while maintaining a linear variation across the layer. The simulated configuration is identical to the actual record holder cell [1,12,13]. The structure is simulated using SCAPS, a solar cell simulation program developed by the University of Gent, affirmed for thin film solar cells, especially for the study of CIGS and CdTe based solar cells [14].

2. Simulation model

The starting point for simulations is the three-layer CIGS baseline solar cells fabricated by Ramanathan et al. and record holding cell of Jackson et al. [1,12,13]. The cell structure can be described as follow: soda-lime glass substrate (3 mm), sputtered molybdenum (500–900 nm), CIGS (2.2–3.0 μm), chemical bath deposited CdS buffer layer (30–50 nm), sputtered undoped ZnO (50–100 nm), sputtered aluminium doped ZnO (150–200 nm) and a nickel/aluminium-grid. A typical structure is shown in Fig. 1.

The simulation software is SCAPS 1D, a solar cell numerical simulator, successfully tested for a variety of CIGS solar cells and proved to give a good analysis [9,15]. In its latest version (SCAPS 2.9) all material properties of alloys with varying composition fraction are computed using the composition value x through one of the implemented laws offered by the user interface: linear, logarithmic, parabolic (two laws), power law, exponential, effective medium and a Beta function. The simulation is performed under global AM1.5 solar spectrum and at ambient temperature of 25 °C conditions. Measurements of photovoltaic parameters are made in the case of zero series and infinite shunt resistances. A summary of used electronic parameters are gathered in Table 1. Input parameters were extracted from literature, either experimental or theoretical data values [6,9,16,17]. In this simulation we take defect state density less than 10^{14} cm^{-3} to account for enhanced CIGS layer quality in accordance with refs. [1,4,15]. The metal work function at back-contact is $\varphi_M = 5.1$ eV (molybdenum) which results in barrier φ_B equals to 0.21 eV. Front and back contacts recombination velocities are fixed at 10^7 $cm.s^{-1}$.

3. Simulation results and discussion

3.1. Uniform band-gap CIGS absorber

Fig. 2 and 3 show photovoltaic parameters of a simulated ZnO/CdS/CIGS solar cells as a function of the CIGS uniform absorber layer band-gap, ranging from 1.01 to 1.68 eV, corresponding to Ga/(In+Ga) (x) ratios variation from 0 to 1. As expected, the behaviour of this cell is in accordance with general trend in photovoltaic cells; low energy band-gap produces