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A comparative study on the performance of Kesterite based thin film solar cells using SCAPS simulation program

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ABSTRACT

A comparative study of thin film solar cells based on CZTS, CZTSe, and CZTSSe (Copper Zinc Tin Sulphur Selenium) absorbers layers were simulated with Cadmium Sulphide (CdS) as buffer layer and Zinc Oxide (ZnO) as window layer using a solar cell capacitance simulator (SCAPS). The influences of series resistance, band to band recombination, defects and interfaces, thickness of (CZTS|CZTSe|CZTSSe) absorber layer, (CdS) buffer layer and transparent conductive oxide layer (ZnO) on the photovoltaic cell parameters were studied in detail. Improvements in efficiency were achieved by changing the back contact metal work function (BMWF) and choosing the flat band option in SCAPS software. Based on the best possible optimisation, an efficiency (η) of 12.03%, 13.16% and 15.77% were obtained for CZTS, CZTSe, and CZTSSe respectively. The performance of thin film photovoltaic devices (TFPV), for Mo back contact before optimisation and the SCAPS simulated values (flat band) after optimisation were described in detail to have in-depth understanding for better design of experiments (DOE) to obtain high efficiency solar cells.

1. Introduction

Thin-film photovoltaic materials [1], such as $Cu(In,Ga)Se_2$ (CIGS) and Cadmium Teluride (CdTe), have attracted great deal of attention for several decades of research, because of their ability to

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produce low cost and high efficiency with large-area thin-film solar cells [2,3,20,22,23]. In response to the high material usage and costs of CIGS materials, a reliable alternative materials such as Cu_2ZnSnS_4 (CZTS), $Cu_2ZnSnSe_4$ (CZTSe), and $Cu_2ZnSn(S,Se)_4$ (CZTSSe), is being extensively studied as a possible alternate absorber material for thin-film solar cells [4,24–26]. They exhibit Kesterite type structure and have their bandgap value close to optimal single junction value (~1.5 eV) with structural similarities to Chalcopyrite ($Cu(In,Ga)Se_2$) solar cells [6]. The bandgap value can be further reduced by alloying CZTS with Se counterpart, and thus, $Cu_2ZnSnSe_4$ (CZTSe) along with $Cu_2ZnSn(S,Se)_4$ (CZTSSe) absorber layers potentially increases the efficiencies of the solar cell [6]. Recently in 2013, Wang et al. [11] demonstrated $Cu_2ZnSnSSe_4$ based solar cells, which demonstrated a record cell efficiency of around 12.6% via a hydrazine pure-solution process. Thus, Kesterite based materials are becoming more competitive in comparison with the matured $Cu(In,Ga)Se_2$, by utilising the most promising and naturally abundant thin film PV absorber material [4–8,27]. Kesterite based absorber layer with a larger band gap (E_g > 1.5 eV) enhances the light absorption and the buffer layer at p/i interfaces, with the extraction of the charge carriers, the open-circuit voltage and the fill factor meliorate the overall performance of the solar cell [7]. The transparent conductive oxide layer (i-ZnO) at the front side of solar cell acts as a down-shifting material, and can generate one low-energy photon for every one incident high-energy photon [13].

In this work, we essentially utilised highly proclaimed simulation program called SCAPS (Solar Cell Capacitance Simulator) a windows-oriented program, developed with LabWindows/CVI of National Instruments at University of Gent. SCAPS is a one dimensional solar cell simulation program developed for cell structures of the CIGS, $CuInSe_2$ and the CdTe family [12]. Several modifications in this software however improved its capabilities to work with crystalline solar cells (Si and GaAs family) and amorphous cells (a-Si and micromorphous Si) [12]. The need for numerical modelling is relevant as the absorber/buffer interface involving hetero-junctions is more complex in nature, for thin film polycrystalline solar cells [8,21]. SCAPS has the largest number of AC and DC electrical measurements which can be calculated in dark and light illumination and also at different temperatures, it includes the open circuit voltage (V_{oc}), short circuit current density (J_{sc}), fill factor (FF%), quantum efficiency (QE%), capacitance frequency spectroscopy $C(f)$, capacitance voltage spectroscopy $C(V)$, generation and recombination profiles, carrier current densities, etc [19]. In view of mass manufacturing to potentially reduce the cost, it is highly desirable to reduce the thickness even further [10]. Simulation has become an essential tool for a detailed understanding, inputs to experimental optimisation and further evaluation to study optical and electrical behaviour of the materials involved. In order to facilitate complete understanding about the performance of CZTS, CZTSe and CZTSSe based thin film solar cell, and also to fabricate cells with champion efficiencies, a detailed analysis of all the layers involved in solar cell have to be evaluated. By utilising this software, an optimised and best possible efficiency values were obtained for CZTS, CZTSe and CZTSSe based solar cells. The standard optical thickness of each semiconductor layers have been varied and tuned to get the best possible efficiency value to compare CZTS, CZTSe and CZTSSe based absorber layers. The influences of series resistance, band to band recombination, defects and interface thickness of (CZTS, CZTSe and CZTSSe) absorber layer, thickness of (CdS) buffer layer and zinc oxide window Layer (ZnO) on the photovoltaic cell parameters were the key parameters studied in detail.

Considering the defects and recombination, even in the most ideal device diode recombination is conceived, either at the layer or at the contact or at the interface, on account that current is converted from hole current at the p-contact to electron current at the n-contact [12]. Kesterite solar cells have high recombination paths when compared with chalcopyrite based devices, because, they are many orders of magnitude higher than the Schottky–Queisser (SQ) limit values [9]. In order to identify where the recombination takes place, one has to ascertain the activation energy of the reverse saturation current [9]. The record Kesterite cell showed activation energy lower than the band gap by 180 meV [9,11].

2. Numerical simulation-SCAPS

SCAPS is a numerical modelling tool aimed at simulation of the properties of semiconductor structures. The model is based on solving the basic semiconductor equations (Poisson equation and the