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Enhancement of output performance of Cu_2ZnSnS_4 thin film solar cells—A numerical simulation approach and comparison to experiments

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ABSTRACT

The formation of stable, low resistance and nonrectifying contacts to Cu_2ZnSnS_4 (CZTS) thin film photovoltaic material are the major and critical challenges associated with its effect over the output performance of fabricated solar cells. The solution of continuity equation in one dimension for a soda lime glass substrates (SLG) |Mo | CZTS | CdS | ZnO:Al cell structure is considered in the simulation of its current–voltage characteristics that is governed by the back contact material, acceptor concentration as well as thickness of the CZTS layer. Our primary simulation shows a 6.44% efficiency of the CZTS solar cell which is comparable to reported experimental data if these parameters are not optimized. However, by optimizing them a simulated conversion efficiency as high as 13.41% (V_{oc}=1.002 V, J_{sc}=19.31 mA/cm^2, fill factor (FF)=69.35%) could be achievable. The solar cell with a back contact metal work function of 5.5 eV, an absorber layer's thickness of 2.68 μm and an acceptor concentration of 5×10^{16} cm^{-3} were optimum. The presented optimization is ideal and subject to experimental verification with a precise control of the process parameters along with reduced surface as well as bulk recombination, secondary phases and thermalization losses.

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1. Introduction

Quaternary semiconductor, Cu_2ZnSnS_4, with a kesterite mineral structure namely the CZTS is a material for meeting the requirements for low cost and eco-friendly thin film solar cells, as none of the elements are scarce in the earth crust and the constituents are non-toxic. In the present era of solar cells, it is necessary to fabricate low cost, high conversion efficiency single junction solar cells without degradation of material properties for widely reliable electricity generation. The kesterite compound, CZTS has been studied by several groups over the past years [1] for its qualification as an earth abundant, cheaper, non-toxic alternative to the binary and quaternary compounds, such as CdTe and CuInGa(S,Se)$_2$ (CIGS) solar cells, respectively [1,2]. The CIGS solar cell conversion efficiency has recently reached up to 20.3% [3], and naturally attention should be paid to CZTS for its associated promises and improving efficiency.

The CZTS absorber layers are very promising material because of their direct optical tunable bandgap in the range 1.4–1.56 eV to exploit the greater magnitude of the input solar irradiance from the spectrum and large absorption coefficient, over 10^4 cm^{-1} [4–6] leading a lower materials usage. However, due to the quaternary phase the structural, crystallographic, and electrical properties can be influenced by stoichiometric composition, which will result in formation of native defects [7]. A champion CZTS solar cell achieved power conversion efficiency of 7.3% which is the record efficiency for electrodeposited CZTS devices [8]. Until recently, the efficiency of 6.7% has been reported for CZTS based solar cells by sputtered deposited material in a 0.15 cm^2 device [6]. Conversion efficiency of 6.81% has been achieved for the solar cell area of 0.45 cm^2 fabricated using the thermal co-evaporation technique [9]. Mitzi et al. and Todorov et al. reported a higher efficiency of 9.7% for CZT(S,Se) deposited by a solvo–thermal deposition technique [1,10]. However, focusing on the Selenium free, pure Sulfur based kesterite compound allows retention of the non toxic absorber and provides a route to higher band gap absorber closer to the optimum bandgap value of 1.45 eV for a single junction solar cell under AM1.5 G radiations [11].

In some previous works, CZTS with specific metal enrichment and introduced defects have been reported [12]. The defects, as well as the smaller grain size of CZTS cause a shorter diffusion length of carriers. The performance in CZTS film is limited by low open circuit voltage (V_{oc}) due to recombination loss with activation energy less than the bulk band gap, high series resistance (R_s), and double diode behavior in the current–voltage characteristics especially in the thicker film [1]. Polycrystalline CZTS based solar cells have shown high series resistance, R_s=4.25 Ω cm^2 and

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low shunt resistance, $R_{sh}=370\,\Omega\,cm^2$ [6]. The higher series resistance and lower shunt resistance of the cells will lead to reducing efficiency by affecting current–voltage (J–V) characteristics. However, light soaking can improve the performance [6]. At the same time, the temperature dependence of CZTS solar cells should be considered as the solar cells performance generally decreases with increasing temperature. It happens due to an increased carrier recombination rates, caused by thermal agitations [1,12].

Modeling current and voltage is widely used in the analysis of single junction solar cells to predict their performance. As CdS/CZTS thin film polycrystalline solar cell is complex in nature, involving heterojunction, the need for numerical modeling in one dimension is relevant. A numerical simulation of solar cell is an important way to predict the effect of various model parameters on the output performance and to test the variability of the proposed structure and materials property. The basic semiconductor equations considered in such a simulation are Poisson's and continuity equations for electrons and holes [13]. Several numerical programs (SCAPS, AMPS, AFORS-HET, PC-1D, Sentaurus and Silvaco-TCAD) which apply these equations have widely been used [14–17] to simulate TFPV devices. The program SCPAS have been employed in our present study, and details of structure and simulation of the device are elaborated in following sections.

2. Device structure and simulation

A solar cell structure of soda lime glass (SLG) | Molybdenum | CZTS | CdS | ZnO:Al | Flat contact was implemented in this study in the SCAPS 2.9.2 environment. Fig. 1 illustrates the vertical cross section of this device. Transparent conducting oxide (TCO) was chosen as front contact, the n-CdS film as the window layer, p-CZTS film as the absorber layer and Molybdenum (Mo) as a back metal on the SLG substrate. The device was considered illuminated with AM1.5 spectrums (1 kW/m^2) from TCO end of the device. The graphical energy band diagrams as model output are shown in Fig. 2 for non-equilibrium condition.

As the hetero-junction formed, the Fermi level of all layers align and all the bands line up accordingly at equilibrium along with the vacuum level. Energy band discontinuity is the major concern for the heterojunction based thin film PV devices as far as the collection of carriers at the metal contacts is concerned. Under illumination, excess free carriers are generated and the Fermi level splits into the quasi-Fermi levels. The separation between the quasi-Fermi levels originates the open circuit voltage in the device.

The device and material parameters used in the simulation which were selected based on literature values, theory, or in some cases reasonable estimation are listed in Tables 1 and 2, specific to the device and materials properties, respectively. The front metal

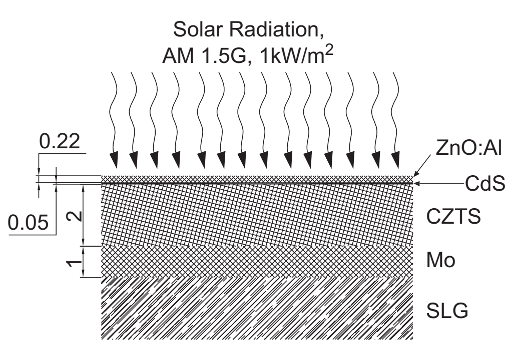

Fig. 1. Structure of the CZTS solar cell used for one dimensional simulation. All geometric dimensions are in micrometers.

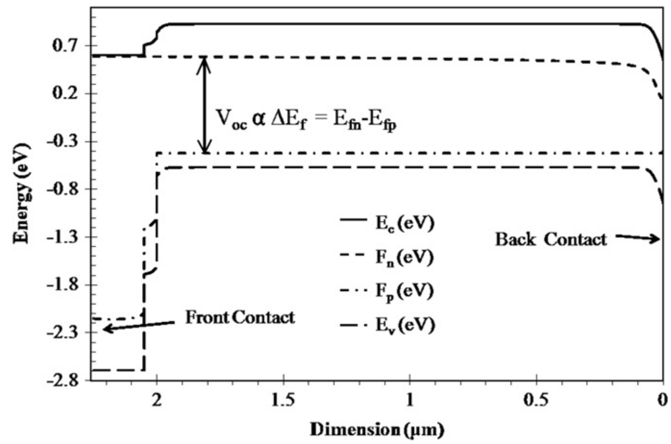

Fig. 2. Graphical representation of the band alignment within CZTS solar cell at nonequilibrium (under illumination). Here ΔE_f, f_n, f_p, E_c and E_v are separations of the quasi-Fermi levels for electrons and holes, quasi-Fermi level corresponding to electrons.

Table 1
Device parameters used in the simulation.

Cell properties	
Cell temperature	300 K
Series resistance, R_s	4.25 Ω cm^2
Shunt resistance, R_{sh}	400 Ω cm^2
Back metal contact properties	
Electron work function of Mo	5 eV
SRV[a] of electron	10^5 cm/s
SRV of hole	10^7 cm/s
Front metal contact properties	
Electron work function	Flat band
SRV of electron	10^7 cm/s
SRV of hole	10^5 cm/s

[a] SRV represents surface recombination velocity.

contact is considered as a standard flat band one and back metal contact is concerned for optimizing the output performance.

In this simulation, the effects of radiative recombination and Auger electron/hole captures have been considered throughout all the cases. The absorption coefficient (α) for the CZTS thin film was considered to be $2.5\times10^4\,cm^{-1}$ [4,5] and the variation of $(h\nu\alpha)^2$ as a function of photon energy, $h\nu$ for CZTS thin film is shown in Fig. 3. Here ν is the photon frequency.

3. Results and discussion

3.1. Basic device simulation based on radiative and Auger recombination

The SCAPS simulation program has been utilized to explore the output performance of the traditional Al:ZnO/CdS/CZTS/Mo solar cell with 5–6 eV of electron work function of back metal contact (M), as well as by varying acceptor concentration of CZTS layer which is function of the Cu/(Zn+Sn) stoichiometric ratio, and the different absorber layer thicknesses. The radiative recombination and Auger electron/hole capture coefficients were considered for existing CZTS thin film layer before pursuing the simulation. The radiative recombination coefficient, B_r depends on the band-gap and whether the semiconductor has a direct or an indirect band-gap. Direct band-gap semiconductors have B_r in the range of 10^{-11}–$10^{-9}\,cm^3\,s^{-1}$, whereas indirect band-gap semiconductors have B_r in the range of 10^{-15} –$10^{-13}\,cm^3\,s^{-1}$ [18]. So far these

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