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Boosting CZTSSe Solar Cell Efficiency by Back Surface Field Layer

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In this work, a simulation of the CZTSSe ($Cu_2ZnSn(S,Se)_4$) solar cell with Al/ZnO:Al/ZnO(i)/CdS/ CZTSSe/Mo structure have been studied using the SCAPS-1D (Solar Cell Capacitance Simulator in one Dimension). The simulation results have been validated with real experimental results. Next, a novel structure is proposed in which a back surface field (BSF) layer is inserted in order to boost the solar cell performance, a CZTSSe layer has been used as (BSF) layer. The efficiency of CZTSSe solar cell increases from 12.3 % to 15.3 % by inserting a BSF layer. Finally, an optimization of different physical parameters (Thickness and doping concentration) of BSF layer has been done, and the optimum values are determined. In this research work, the proposed structure of CZTSSe solar cells with optimum parameters showed higher functional properties, The maximum value of efficiency achieved was 16.98 % with J_{sc} = 36.31 mA/cm², V_{oc} = 0.69 V, and FF = 69.60% under 1.5G AM illumination.

Keywords: BSF, CZTSSe, Solar cell, SCAPS-1D, Thin film.

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1. INTRODUCTION

The world needs power more and more in all domains, as a result of reduction in conventional energy reserves, looking for alternative source of clean energy, environment friendly, cost effective and sustainability became a burning priority, researchers focus mainly on solar energy which is the most promising, powerful , reliable and abundant form of renewable energy that serves as an alternative resource of energy [1-3]. Researchers have employed several materials such as CdTe, CIS, CIGS to achieve high efficiency solar cells with low cost [4]. However, Cadmium (Cd) is a toxic element and heavy metal that is polluted the environment. The lack of materials in Telluride (Te), Indium (In) and Gallium (Ga) in earth increase the price of these materials day to day [5]. Consequently, several groups of researches were motivated to introduce new environmentally and friendly materials [4].

Thin-film solar cells based on $Cu_2ZnSn(S,Se)_4$ (CZTSSe) are an interesting alternative to other thin-film photovoltaic technologies, due to promising performances combined to earth-abundant elements, it's have useful band gap energies (E_g) of 1.0-1.5 eV and high absorption coefficients exceeding 10^4 cm^{-1}. However, CZTSSe, with a low power conversion energy (PCE of 12.6 %), in comparison with CdTe (PCE of 21.5 %) and CIGS(PCE of 21.7 %), CZTSSe still need improvement[6]. To date, the major limitation of CZTSSe solar cells is the open-circuit voltage (V_{oc}), whereas, the causes of this problem has been a subject of intense debate [7]. One of the promising technics for enhancing the power conversion energy (PCE) of solar cells is by using a back surface field (BSF) which is to make the back/bottom heavily doped acting as a rear pushing force to push the minority carrier to the front (depletion area)[8], also, it minimizes the rear recombination of the solar cell, which allow to improve electrical characteristics of the solar cells, especially, the open circuit voltage. The materials selected for the realization of this layer must have a mesh parameters close to the mesh parameters of the base layer, a high concentrating doping of the order of 10^{18} cm^{-3} [9] and good transparency to photons for the lower cell (Bottom cell), if this layer is applied in a tandem solar cells structure [10]. In this research paper, the boosting of CZTSSe solar cells efficiency is proposed by adding a back surface field (BSF) layer, the focused objective is to enhance the electrical parameters of CZTSSe solar cells, open voltage V_{oc} and short current circuit J_{sc}. This enhancement conducts to boost the electrical efficiency (η) of the solar cell. At first, the one-dimensional simulator SCAPS-1D is used to analyze numerically the performances of the design of CZTSSe solar cells without back surface field (BSF) and compared with the previous reported experimental results[6], then we analyze the new proposal design of CZTSSe solar cell with back surface field layer. Finally an optimization of the physical properties of the proposal BSF layer (Thickness and carrier concentration) will be done.

2. DEVICE STRUCTURE AND SIMULATION

In this study, we consider the structure of thin film CZTSSe for simulation which were made by Yang et al [6], this cell was prepared with several ratios of Se/SeS_2, an electrical efficiency of 12.3 % was achieved with an energy gap of 1.097 eV corresponding to 38 % of Se/SeS_2 ratio [6].

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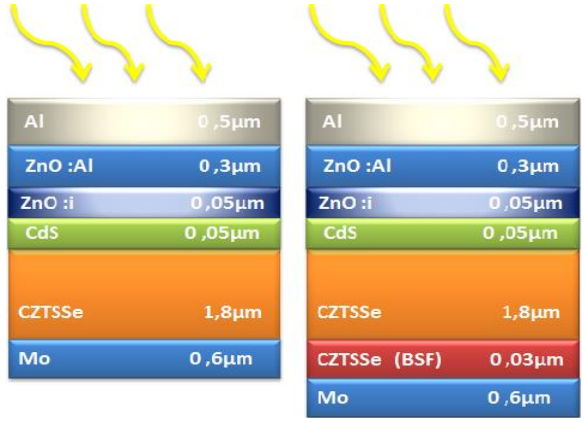
2.1 The CZTSSe Solar Cell Structure

The schematic structure of CZTSSe solar cell is shown in Fig. 1a, it consisted of the following layers: Window layer which composite of Aluminum doped zinc oxide (ZnO: Al) and intrinsic zinc oxide (ZnO-i), a Buffer layer represented by Cadmium Sulphide(CdS) and at the end Absorber layer made by CZTSSe. A Molybdenum (Mo) layer is used as back contact. This structure is assumed to be deposited on a Soda Lime Glass (SLG).



a b

Fig. 1 – Schematic diagram of the studied CZTSSe structure: (a)-Experimental design [6], (b)-the proposed design

2.2 Simulation and Validation

Numerical simulation is a necessary tool for analysis, comprehension and enhancing of solar cells performances, it makes the examination and optimization of the parameters of the cell easier and without fabrication[11]. The simulation program used for modeling of thin film solar cells in particular, must be able to solve the basic semiconductor equations. The basic equations are: the Poisson equation, relating the charge to the electrostatic potential φ and the continuity equations for electrons and holes [10-11], which are denoted below with constitutives equations 1, 2 and 3:

$$\frac{\partial}{\partial x}\left(\varepsilon_0\varepsilon_r\frac{\partial \Psi}{\partial x}\right)=-q(p-n+N_D^+-N_A^-+\frac{\rho_{def}}{q}), \quad (1)$$

$$-\frac{\partial J_n}{\partial x}-U_n+G=\frac{\partial n}{\partial t}, \quad (2)$$

$$-\frac{\partial J_p}{\partial x}-U_p+G=\frac{\partial p}{\partial t}, \quad (3)$$

where Ψ is the electrostatic potential, $\varepsilon_0, \varepsilon_r$ are the permittivity of vacuum and semiconductor, n and p are the free carrier concentration, N_D^+ and N_A^- are the density of ionized donors and acceptors, ρ_{def} is the charge density of defects, q is the magnitude of the charge of an electron, G is the generation rate, J_n and J_p are the electron and hole current density respectively, U_n and U_p are the recombination rates for the electrons and holes respectively.

The charge carrier transport is described by the drift and diffusion is expressed by equations 4 and 5 as:

$$J_n=-\frac{\mu_n n}{q}\frac{\partial E_{Fn}}{\partial x}, \quad (4)$$

$$J_p=-\frac{\mu_p p}{q}\frac{\partial E_{Fp}}{\partial x}, \quad (5)$$

where E_{Fn}, E_{Fp} are the quasi-Fermi level for the electrons and holes respectively [14].

Table 1 – Parameter set for the simulation of the CZTSSe solar cell

Layer	ZnO:Al	ZnO-i	CdS	CZTSSe
Thickness (nm)	300	50	50	1800
Electron affinity (eV)	4,4	4,4	4,2	4,1
Band gap (eV)	3,3	3,3	2,4	1,096
Dielectric permittivity (relative)	9	9	10	13,6
Effective conduction band density (cm^{-3})	2,2E18	2,2E18	2,2E18	2,2E18
Effective valence band density (cm^{-3})	1,8E19	1,8E19	1,8E19	1,8E19
Electron mobility (cm^2/Vs)	1E2	1E2	1E2	1E2
Hole mobility (cm^2/Vs)	2,5E1	2,5E1	2,5E1	2,5E1
Electron thermal velocity(cm/s)	1E7	1E7	1E7	1E7
Hole thermal velocity (cm/s)	1E7	1E7	1E7	1E7
Doping concentration of acceptors (cm^{-3})	0	1E18	0	1E15
Doping concentration of donors (cm^{-3})	1E18	1E18	1E17	0

In this study, CZTSSe solar cell structure is modeled by using SCAPS-1D simulator, highly proclaimed simulator, the program developed at the Electronics and Information Systems Department, Gents University, Belgium[6, 8]. This program is designed to simulate the electrical characteristics as well as the spectral response of thin film hetero-junction solar cells[12]. The solar cell can be modeled in one dimension across, using at maximum seven layers for their description. SCAPS-1D Simulation program requires large amount of physical and optical parameters of semiconductor material [15] which includes; band gap (E_g), electron affinity (χ), dielectric permittivity (ε), conduction band density of states (NC), valence band density of states (NV), electron thermal velocity (V_{thn}), hole thermal velocity (V_{thp}), electron mobility (μ_n), hole mobility (μ_p), donor density (NA), acceptor density (ND) and Absorption coefficient (α). The physical parameters used in

this work for different material layers were all cited from experimental study [6] and literatures[8, 11], which are summarized in Table 1. The simulation of CZTSSe solar cell had been done under a global solar irradiance AM 1.5G (1000 W/m²) and an operating temperature of 300 K.

2.3 Results and Discussion

The simulation of the CZTSSe solar cell using the parameters of the solar cell presented in table.1 gave an efficiency of 12,4% (V_{oc} = 0.7447 V, J_{sc} = 24.786 mA/cm², FF = 65.19 %). These results are in agreements with the experimental results in reference [6]. The comparison between experimental and simulation results of J-V curves and quantum efficiency of CZTSSe solar cell are shown in Fig. 2 and Fig. 3 respectively. We notice a good agreement between simulation and experimental results curves. Table. 2 summarizes the obtained electrical parameters of simulation results in comparison with experimental data of reference [6].

Table 2 – Experimental and Simulation characteristics of the CZTSSe solar cells

	V_{oc} (V)	J_{sc} (mA/cm²)	FF (%)	η (%)
Experimental data	0.520	34.64	67.2	12.1
Simulation data	0.532	33.75	68.9	1.4

3. BOOST THE PERFORMANCE OF CZTSSE SOLAR CELLS WITH A CZTSSE LAYER AS BSF

After the validation of the simulated model (using SCAPS-1D) with experimental results[6], a proposed solution is given in order to enhance the performances of the studied solar cell. A highly doped thin layer with CZTSSe material is added under CZTSSe absorber layer, it plays the role of BSF, the schematic diagram of the proposed structure is presented in Fig. 1b.

The Back Surface Field (BSF) layer is used to minimize rear recombination of the cell. It is obtained by abrupt transition of the doping on the rear face of the solar cell in the zone of the ohmic contact.

The introduction of this layer makes possible to improve the electrical characteristics of the solar cell, in particular the open circuit voltage (V_{oc}) by reducing the dark current. The minimization of the recombination on the back side of the cell helps to improve the spectral response for the long wavelengths. Moreover, it brings an increase in the open-circuit voltage (V_{oc}) and the short-circuit current density (I_{SC}). The excess carriers thus created in the vicinity of the base, instead of recombining are pushed back to the space charge region of the junction[16].

The comparisons between simulated J-V curves of the proposed designed cell (solar cell with BSF) with the previous case (solar cell without BSF) and the experimental results are shown in Fig. 2. It's obvious, compared with same structure without BSF layer (simulated and experimental), the results of this proposed model with BSF show more efficient performance with higher solar cell efficiency. The functional parameters of these solar cells are indicated in Table 3, it is completely clear from it that both parameters V_{oc} and J_{sc} are increased, making an enhancement in efficiency of the solar cell.

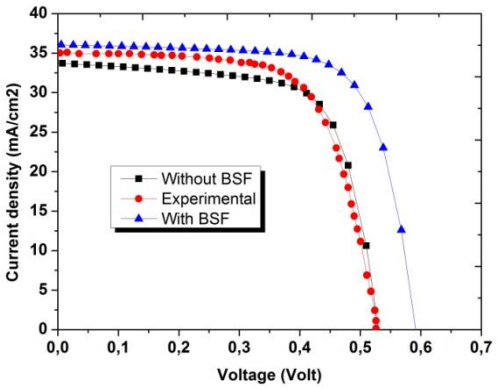


Fig. 2 – J-V characteristics of CZTSSe solar cell with BSF and without BSF (experimental and simulation)

The quantum efficiency as a function of wavelength for these solar cells is exhibited in Fig.3, it indicates a high performance achieved with CZTSSe solar cell with BSF considering the same structure without BSF. The enhancement is observed for the highest wavelength.

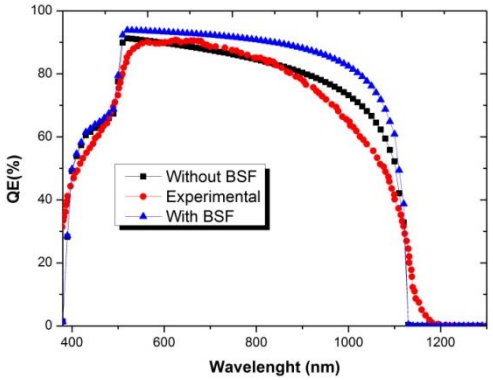


Fig. 3 – Quantum efficiency curves for CZTSSe solar cell with BSF and without BSF (experimental and simulation)

From Table 3, we notice an enhancement of 26.44 % in the conversion efficiency of the proposed cell (with BSF) in comparison with experimental results of the solar cell and the simulated model (without BSF).

Table 3 – Functional parameters of the CZTSSe solar cells without and with BSF.cells

Cell		V_{oc} (V)	J_{sc} (mA/cm2)	FF (%)	η (%)
BSF	Simulation	0.59	36.06	71.29	15.3
No BSF	Experimental	0.520	34.64	67.2	12.1
	Simulation	0.532	33.75	68.9	12.4

4. OPTIMISATION OF THE BSF PARAMETRES

4.1 Effect of CZTSSe BSF Layer Thickness

The effect of BSF layer thickness on the electrical performances of CZTSSe solar cell is studied in this

part, Fig. 4 and Fig. 5 show the variation of J_{sc}, V_{oc}, η and FF as a function of the BSF thickness. It is observed that these parameters are strongly dependent on BSF layer thickness. As we are seeing from the Fig. 4 and Fig. 5, J_{sc}, V_{oc}, η and FF are significantly increased with increase in BSF thickness, J_{sc} is saturated at 30 nm (0.03 μm) thickness. Whereas for V_{oc}, it still increasing until saturation thickness at 50 nm (0.05 μm) with maximum efficiency achieved of 15.65%. The Fill Factor is slightly affected to BSF thickness variation, it varies in the range of 69.02-71.3%.

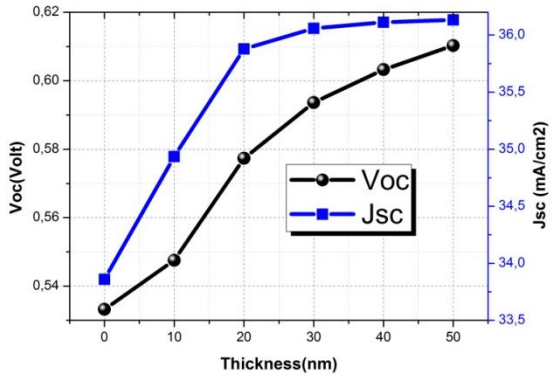


Fig. 4 – Variation of Short Circuit Current and Open circuit voltage as a function of BSF thickness

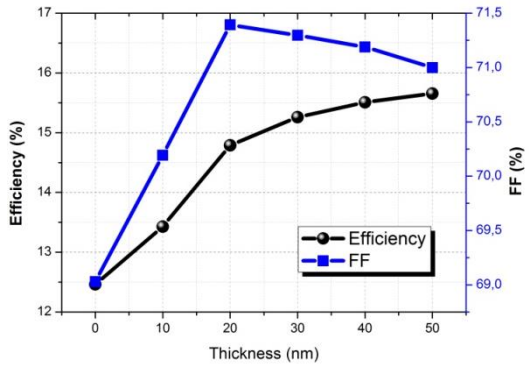


Fig. 5 – Variation of Fill Factor and Efficiency as a function of BSF thickness

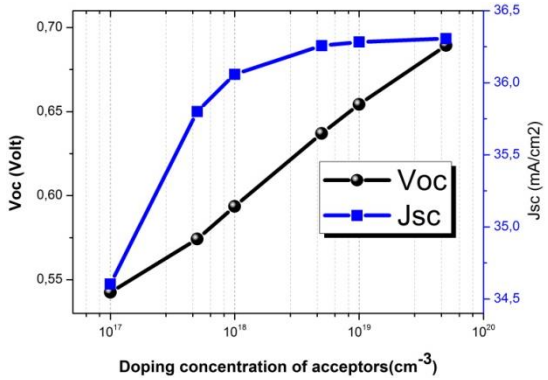


Fig. 6 – Variation of Short Circuit Current and Open circuit voltage as function of BSF doping concentration

4.2 Effect of CZTSSe BSF Layer Doping Concentration

In this part, the numerical analysis has been done to investigate the doping concentration of BSF layer effect on the functional properties of CZTSSe solar cell. The doping concentration is varied for BSF layer in the range of [1E17-5E19 cm^{-3}] as shown in Fig. 6 and Fig.7. The increase of BSF doping concentration causes the increase of J_{sc}, V_{oc}, η and FF of the solar cell, Fig. 6 shows that J_{sc} and V_{oc} rise sharply with the increase of doping concentration, but the V_{oc} increases gradually after 1E18 cm^{-3}. From Fig. 7 we note that η and FF increases gradually whereas FF decreases after 1E18 cm^{-3} with maximum efficiency achieved of 16.98% at 5E19 cm^{-3} doping concentration.

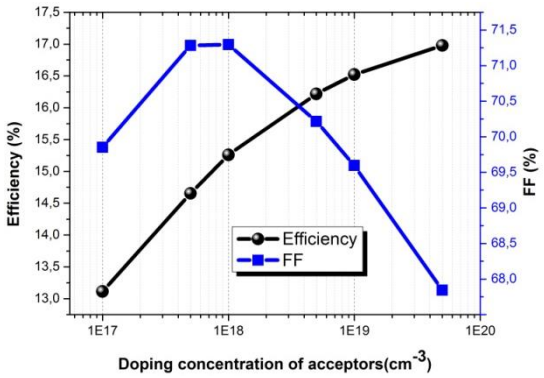


Fig. 7 – Variation of Fill Factor and Efficiency variation as function of BSF doping concentration

5. CONCLUSION

In this paper we reported an effective method to increase the efficiency of CZTSSe solar cell by inclusion of a back surface field (BSF) layer, at the beginning and in order to improve the accuracy of simulated model's results, a simulated CZTSSe solar cell model without BSF was validated with published experimental data. The next step in this work is enhancing the CZTSSe solar cell performance by introducing back surface field layer represented by CZTSSe material. The efficiency of CZTSSe solar cell is increased from 12.3 % to 15.3% (J_{sc} = 36.06 mA/cm², V_{oc} = 0.59V, FF = 71.29%) with an increasing of 26.44% in comparison with experimental results. At the end, by the aim of making functional parameters of CZTSSe solar cells as high as possible, an optimizing of thickness and doping concentration of the BSF layer is carried out from simulation results. A hight functional parameters achieved, an efficiency of 16.98% (V_o = 0.69V, J_{sc} = 36.31 mA/cm²) with a rising of 40% in comparison with experimental results at doping concentration value of 5E19 cm^{-3}, whereas the maximum value of fill factor is 71.39 % at 0.05 μm thickness. The quantum efficiency increased in the large wavelength (range of 650-1000 nm), the proposed model of solar cell with such characteristics has better conversion efficiency compared with the work reported so far.

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