A Study to Investigate High Efficiency CZTS Based Solar Cells with SCAPS-1D

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***Abstract*—It is found in recent studies that researchers are focusing more on CZTS types solar cells because of the competent characteristics of its constituent material than CIGS, Silicon, CdTe solar cells. In this study high-efficiency Cu_2ZnSnS_4 (CZTS) solar cells with ZnS antireflection coating have been simulated using SCAPS-1D. CZTS based thin-film is getting concerned with promising material for implementing a different photovoltaic application with advantages like low manufacturing cost, high efficiency, and environment friendly. We have tried to optimize the absorber layer of the MoS_2O/CZTS/CdS/ZnO/n-ITO/ZnS solar cells. In this model, different parameters such as fill factor, open-circuit voltage, efficiency and short circuit current density (J_{SC}) have been observed with different bandgaps and absorber layer thickness for better results. After the simulation, the best observed efficiency is 16.03%, while FF, J_{SC} & V_{OC} are 76.19, 32.696217, and 0.6435 for different bandgaps, respectively.**

Keywords— CZTS, Thin film, ZnS, Simulation, SCAPS-1D

I. INTRODUCTION

Among cadmium telluride (CdTe), amorphous silicon (a-Si), $CuInGaS_2$, $CuInGaSe_2$ (CIGS), Cu_2ZnSnS_4 (CZTS) types of thin films solar cell, nowadays, researchers are focusing on CZTS based solar cells. Though CIGS, Si, CdTe solar cells are more efficient solar cells found ever, due to some detrimental effect of these cells on the environment, high manufacturing cost and scarcity of Cadmium on earth are deterring, precluding researchers from continuing research. Also inspiring researchers to look forward on other types of solar cell which can resolve these problems. Still, researchers have found that CZTS is the most promising material used as an absorber layer, more environmentally friendly, cost-efficient, and abundant in nature. In an experimental study, when the absorber layer is CZTS with ZnO: Al, M. Djinkwi Wanda, S. Ouédraogo found an increased efficiency of 8.4% [1]. Farjana Jhuma, Marshia Shaily, found efficiency of 11.20% using CZTS as an absorber layer and optimizing different layers [2]. Ashkan et al. used ITO/TiO2 with CZTS solar cells and found an efficiency of 11.06% [3]. In another study, Shahram et al. found efficiency of 15.6% at his CZTSSe solar cell that used the bandgap grading model [4].Swati Tripathi et al. observed efficiency of 15.68 % at his numerical analysis study with CZTS based solar cells and a hybrid buffer layer [5].

In this work, ZnS has been used as antireflection coatings; thus, a reflection of light can be minimized, and absorption of light can be increased. Another layer in this structure mentioned as CZTS works as an absorber layer experimented with by varying bandgap via different methods. This layer coated over deposition on the Molybdenum Sulfide (MoS_2), which is a glass substrate. The high absorbance and low absorbance are found in the light absorption of any thin-films solar cells. Absorbance increases in nature, whether it is inferior in the visible and infrared regions in case of ultraviolet rays having a range of (0.36-0.45 μm) [6] [2] [7].

II. SIMULATION SOFTWARE

SCAPS is a program software that is designed to simulate 1-D solar cells and to observe different characteristics of solar cells, which was invented by the Department of EIS, University of Gent, a Belgian university [8]. This simulation program has the facility to control material properties [9]. Layer parameters such as thickness, bandgap, dielectric permittivity, hole-electron mobility, etc., are used as input in SCAPS-1D [2], [13-15]. The input parameters of any model can be manipulated by this program, and it can quantify changes in Voc (open-circuit voltage), Jsc and quantum efficiency. Several solar cells simulation program software is available, such as photonic computer one dimensional (PC-1D), one dimensional Solar Cell Capacitance Simulator, a program for simulation of heterojunction solar cell (AFORS-HET), analysis of silicon amorphous (ASA), etc. Among all of these, SCAPS-1D is used widely because of its handy features, different windows that show all parameter results decorously, and a collaborative agreement of thin film solar cells. Hence in our study, we used SCAPS-1D [6],[10]. In this study, we simulated a CZTS solar cell using SCAPS-1D to determine different solar cell parameters, including efficiency by varying bandgap of the absorber layer. These DC and AC electrical parameters are efficiencies, C-V, J-V, quantum efficiency, etc. SCAPS calculates these parameters at different illumination moods (light, dark) at various AM solar spectrum ranges. SCAPS also calculates other parameters like generation-recombination profile, capacitance-voltage spectroscopy, capacitance frequency spectroscopy, electrical shunt resistance, and carrier current density [11],[12]. At AM 1.5 solar spectrum experiment was done to characterize the solar cells. Where CZTS was used as absorber layer, ZnS as buffer layer and CdS as ARC layer. Optical bandgaps and electrical properties of these materials are very suitable to increase our structure's efficiency so that these layers were used to have a practical solar cell.

III. THE BASIC STRUCTURE OF THE SIMULATED MODEL

This study is related to CZTS thin-film, and it is already mentioned in the introduction that the absorber layer of our structure is CZTS. The design started with a glass substrate made of soda-lime. A thin MoS_2O layer of the optimum thickness measured in nm was used over the absorber layer to avoid the high series resistance. In CZTS solar cells, this layer is formed in the absorber precursor (ZnS or SnS) by a reaction of Molybdenum (Mo) with sulfur [16]. The layer next to back contact is the absorber layer. CZTS was used as the absorber layer material, many other materials like CIGS, CdTe, and Si can also be used as absorber layers, but due to the economic goal here, CZTS was used. Hole electron pairs are created in absorber layer, where photons are absorbed. The absorber layer is considered the most crucial layer of this solar structure. The next layer used over the CZTS layer is a buffer layer. Several materials can be used as a buffer layer. Most commonly, CdS, $Cd_{0.4}Zn_{0.6}S$, or ZnS is used in solar cells. It can be seen from Fig.1 CdS was used as a buffer layer in the structure. Band alignment betwixt CZTS absorber layer and the window layer is provided by this buffer layer. Afterward, a window layer on top of the buffer layer, cost-efficient, abundant ZnO of favorable thickness in nm was used. The light scattering is enhanced by this window layer. It enables efficient sunlight to increase the number of photons in the buffer and absorber layers [17]. Over the window layer, another layer was used, with a thickness of near 60 nm, which is the transparent conducting film n-ITO. Which was used to supply high mobility leading to an improvement in visible absorption to acquire a lower sheet resistance [18]. Finally, over the TCF, a layer of antireflection coating (ARC) was used. Generally, ARC can be made of different materials like MgF_2, ZnS, ZnO, SiN_3, SiC, TiO_2, ZnO: Al, ZnO: B, SiO_2, etc. The outermost layer ZnS is used as an ARC layer, which reduces the rate of light reflection. Sunlight power of 1000 W/m^2 with AM 1.5 spectrums has been illuminated from the front contact.

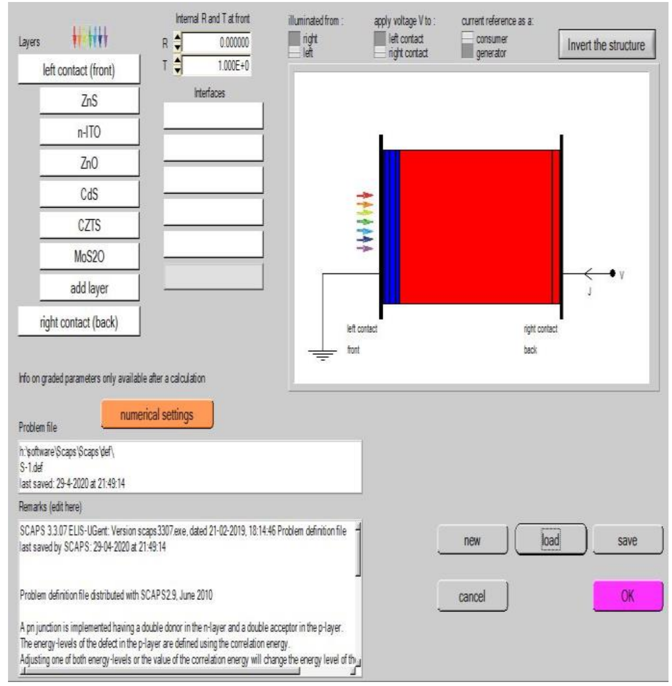

Fig. 1. Simulated structure on SCAPS definition panel

IV. RESULTS AND DISCUSSION

A. *A variation on CZTS solar cells performance concerning Bandgap & Thickness*

For any semiconductor, an electron bandgap is one of the material properties. The energy that is essential to excite an electron from VB to CB is called a bandgap. We know the conduction band is filled with holes, and the valence band is filled with an electron. Then the energy differences between these bands provide the value of bandgap [19].

There are several kesterite-based semiconductors, and CZTS is one of them. Typically, the energy bandgap of this kesterite absorber layer is around 1.4-1.5 eV. The modification of the bandgap property of CZTS material can be skillfully done through alloying with different types of dopant elements like

TABLE. 1. PHYSICAL PROPERTIES OF DIFFERENT MATERIALS

Parameter	**MoS_2O**	**CZTS**	**CdS**	**ZnO**	**n-ITO**	**ZnS**
Thickness (nm)	100	100-2000	50	80	60	30
Band gap (eV)	1.7	1.5	2.4	3.3	3.6	3.68
e affinity (eV)	4.2	4.5	4.5	4.6	4.1	4.13
Permittivity	13.6	10	10	9	10	8.28
CB effective density of states (cm^{-3})	$2.2x10^{18}$	$2.2x10^{18}$	$2.2x10^{18}$	$2.2x10^{18}$	$2.2x10^{18}$	$1.7x10^{18}$
VB effective density of states (cm^{-3})	$1.8x10^{19}$	$1.8x10^{19}$	$1.8x10^{19}$	$1.8x10^{19}$	$1.8x10^{19}$	$2.4x10^{19}$
Electron thermal velocity ($cm\ s^{-1}$)	$1x10^7$	$1x10^7$	$1x10^7$	$1x10^7$	$1x10^7$	$1x10^7$
Hole thermal velocity (cm^{-1})	$1x10^7$	$1x10^7$	$1x10^7$	$1x10^7$	$1x10^7$	$1x10^7$
Electron mobility (cm^2/V_s)	100	100	100	100	50	25
Hole mobility (cm^2/V_s)	25	25	25	25	75	70
Shallow uniform donor density, ND (cm^{-3})	0	$1x10^1$	$1x10^{18}$	$1x10^{18}$	$1x10^{19}$	$1x10^{19}$
Shallow uniform acceptor density, ND (cm^{-3})	$1x10^{16}$	$2x10^{14}$	0	0	0	0
Defect type	-	Donor	Acceptor	-	-	-
Defect density (cm^{-3})	-	$1x10^{13}$	$6x10^{16}$	-	-	-

Se, Cd, Ge, Ni, Mg, Ag, or Co [20]. For instance, alloying CZTS with Se plays down its bandgap unto 1eV. In other words, changing the ratio of S and Se in the CZTS reduces its bandgap. This band-gap engineering's main reason is to separate carrier recombination and current generation mechanisms in these absorber layers.

In this paper, we discussed the consequence of changes in bandgap and thickness of the CZTS absorber layer on solar cells efficiency. The bandgap values of the CZTS layer was taken as 1.1eV to 1.5eV. In Fig. 2.1 and 2.2, the QE and J-V characteristics of our model are shown.

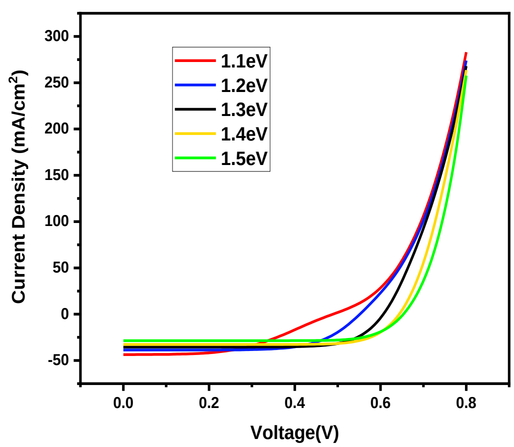

Fig. 2.1 J-V characteristic curves for different Bandgap (eV) of CZTS.

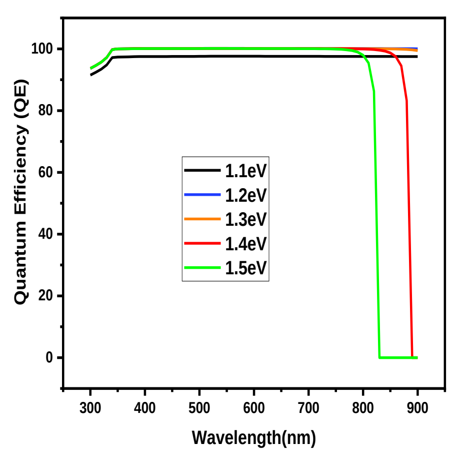

Fig. 2.2 QE curves for different values of Bandgap of CZTS.

Fig.2.1 shows the J-V characteristic graph for different Bandgap (eV) of CZTS. We can see that current density increases with the increase in voltages. When the bandgap is minimum current density is higher, and when the bandgap is higher current density is minimum. We can conclude from the fig. 2.1 that current density is inversely proportional to the bandgap. The highest value and lowest values curves are indicated in the graph by red and green color. From 0.4 voltage there is seen a sharp rise in current density for each bandgap values. Fig. 2.2 shows the QE curves for different values of Bandgap of CZTS. Quantum efficiency has a great fall after a definite range of wavelengths. For each bandgap values, quantum efficiency starts falling from near about 800nm of wavelength, seen from the QE curves

At different bandgaps, simulated different solar cell parameters such as J_{SC}, FF, V_{OC}, and η are depicted in Table-2.

TABLE. 2. SIMULATED RESULTS FOR DIFFERENT BANDGAPS.

Bandgap	Voc (V)	Jsc (mA/cm^2)	FF(%)	η(%)
1.1	0.4887	43.611883	47.91	10.21
1.2	0.5519	38.70935	66.32	14.17
1.3	0.6066	35.495347	73.55	15.84
1.4	0.6435	32.696217	76.19	16.03
1.5	0.6532	28.561207	76.4	14.25

The various parameters that we found for different ranges of thickness of our model's CZTS layer are displayed in Table-3.

Dissimilitude of these solar cell parameters have been plotted in Fig. 3.1,3.2,3.3 and 3.4 for different bandgaps and in figures 4.1, 4.2, 4.3, and 4.4 for different thicknesses of the CZTS layer. The thickness range of the CZTS layer differed from 250nm to 2000nm.

TABLE. 3. SIMULATED RESULTS FOR DIFFERENT THICKNESS.

Thickness(nm)	Voc(V)	Jsc(mA/cm^2)	FF(%)	η(%)
250	0.6385	25.476532	76.32	12.42
500	0.6449	29.788541	76.72	14.74
750	0.6461	31.268626	76.62	15.48
1000	0.646	31.919945	76.52	15.78
1250	0.6455	32.264283	76.44	15.92
1500	0.6449	32.471648	76.36	15.99
1750	0.6442	32.603898	76.27	16.02
2000	0.6435	32.696217	76.19	16.03

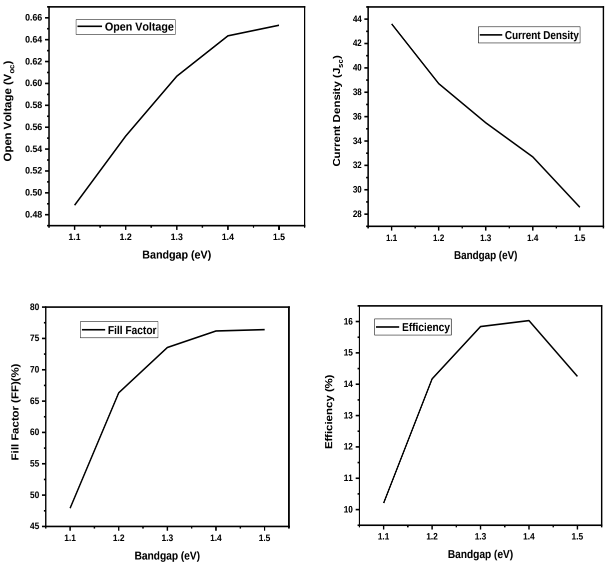

Fig.3 Variation of (3.1) V_{oc}, (3.2) J_{sc}, (3.3) FF, and (3.4) ɳ vs. Bandgap of CZTS layer..

V_{oc} & bandgaps are almost linearly related, which was also observed in Fig.3.1, where, along with the bandgap increases from 1.1eV to 1.5eV, the open-circuit voltage, i.e., Voc also increases [21]. In Fig. 3.1, short circuit current decreases when there is an increase in bandgaps from 1.1eV to 1.5eV. Here, the absorption rate within the CZTS layer decreases with the rise in bandgaps, which is why Jsc gets reduced [22]. By comparing fig. 3.1 and 3.2, it can be seen that the optimum value of the bandgap of CZTS is 1.4eV. A decrease in the absorption within this layer increased Voc and reduced Jsc and [21]. The values of fill factor (FF) increase with the values of bandgaps from 1.1 to 1.5eV. This is the reason why the optimum bandgap value is 1.4eV. FF and efficiency results are shown in Fig. 3.3 and 3.4, respectively. Fig. 3.3 shows, with the rise in bandgaps of the absorber layer, the fill factor increases. This happens due to the rise in hole density [22]. This is also the same for efficiency up to 1.4. That can be seen from Fig. 3.4, where efficiency also increases with the increase in bandgaps.

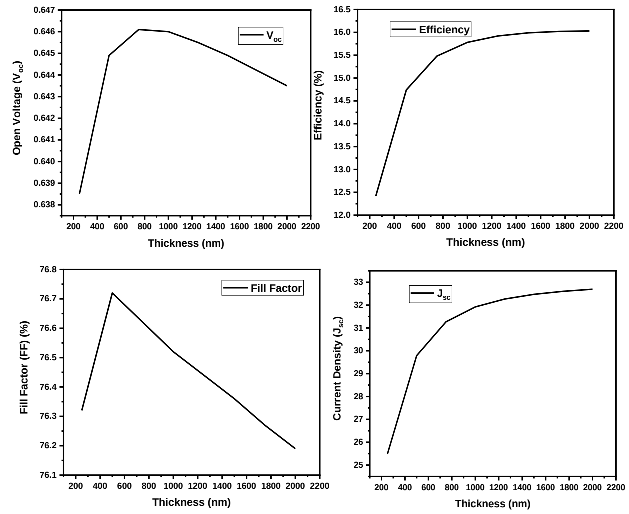

Fig.4 Variation of (4.1) Voc, (4.2) Jsc, (4.3) FF, and (4.4) ɳ vs. Bandgap of CZTS layer.

Fig.4 shows how solar cells' different parameters vary with the CZTS layer's extended thickness. Fig.4.1 shows the Voc, which get increased with the increase in thickness up to 800nm almost. Similarly, other parameters, like current density and efficiency, also increase with the enlargement in thickness, shown in fig 4.2 and 4.3, respectively. With the increase in thickness, efficiency also increases. From fig.4.4, it is clear that the rate of increasing efficiency is sluggish in manner. After 1000nm, if the thickness is doubled, the efficiency only increases by 0.25%, which increases the manufacturing cost but not the efficiency on that level. When the thickness is 2000mm, the highest efficiency of our model was observed. In Fig. 4.4, it is shown that how fill factor gets changed with the different values of thickness. Concisely, Fig. 4 shows the variation of CZTS solar cell efficiency with the absorber layer's diverse range of thickness.

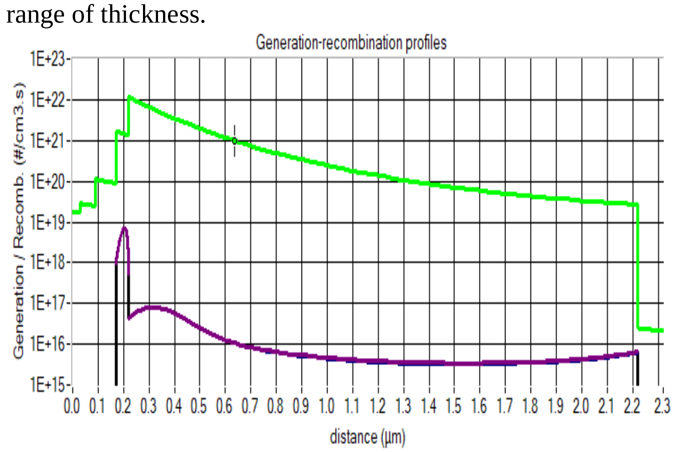

Fig.5 Generation and recombination rates of the CZTS thin-film.

Fig. 5 shows the curves of recombination rates and carrier generation of CZTS solar cells concerning position at 300 K. With the increase in bandgaps, recombination rates, and carrier generation increases. ARC layer ZnS improves the absorption rates. Hence, generation and recombination rates also get increased.

V. Conclusion

In this study, efficiency of CZTS solar cells with ZnS antireflection coatings was investigated by using SCAPS-1D. ARC layer ZnS was used for better light absorption, which is for better generation and recombination rates. CZTS was used as absorber layer. By varying bandgaps and thickness of the absorber layer, performances were investigated. Different parameters of solar cell such as open circuit volt., Jsc, Fill Factor, and efficiency were also investigated. When the bandgap of the absorber layer was 1.4eV, the best efficiency of 16.03% was observed. When, absorber layer thickness was 2000nm, Voc, Jsc, FF, and η were 0.6435 V, 32.696217 mA/cm^2, 76.19%, and 16.03% were observed, respectively. But considering the manufacturing cost, we suggest 1000nm will be most effective with sacrificing only 0.25% efficiency. Therefore, we conclude that for the CZTS layer, the optimum value of bandgap is 1.4eV, and thickness is 1000nm. All these simulations provide significant results for CZTS based solar cells. This will work as a guide for future research to fabricate CZTS absorber based solar cell with ZnS ARC layer.

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