Investigation of Different Materials as Buffer Layer in CZTS Solar Cells Using SCAPS

Md. Noumil Tousif, Sakib Mohammad, A. A. Ferdous, and Md. Ashraful Hoque

Abstract—**Cadmium sulfide (CdS) is widely used as buffer layer of Cu_2ZnSnS_4 (CZTS)-based thin film solar cell. Due to its toxicity, its alternatives are being explored. In this work, with an attempt to find an alternative to Cadmium sulfide, electrical performances of solar cell with different buffer layers were simulated and recorded. Simulation was carried out with Solar Cell Capacitance Simulator (SCAPS). As buffer layer, other than Cds; Zn(O,S), ZnS, ZnSe, InS and MoS_2 were separately used. Zinc compounds are cheap, eco-friendly and they have relatively higher band gap, making them suitable candidate for replacing CdS. Zn(O,S) and ZnS yielded good results with conversion efficiency of 10.28% and 9.82% respectively. This result is favorable for cost-effective fabrication of highly efficient thin film solar cell.**

Index Terms—**Buffer layer, CdS, CZTS, InS, MoS_2, SCAPS, Zn(O,S), ZnSe, ZnS.**

I. Introduction

In the present state of Solar cells, it is highly recommended to fabricate low cost, high energy conversion efficiency solar cells [1] We have used most of our fossil fuels and by the end of this century, all of it will be depleted [2]-[4] Hence we have to find an alternative source of energy and renewable energy i.e Solar energy is the best option amongst the rest.

Primarily, there are two types of solar cells; thin type & bulk type. Being cheaper in price, thin type solar cell became much popular than the other type. Among them CdTe (Cadmium Telluride) and CIGS (CuInGa(S,Se2)) solar cells have the highest uses & the efficiency. [5], [6]. Although in the last decade, CdTe has gained much interest as an absorber layer for having the maximum energy conversion efficiency of 17.3% [7] and CIGS solar cells reached around 20% [8] of energy conversion efficiency, having been found the toxic materials in their constituents, these are not eco-friendly. And also these aren't earth abundant but costly on the other hand. By considering environment friendliness and abundancy in earth's crust and the cost effectivity, CZTS is the best possible option for using it as an absorber layer in Solar Cells. Thin film Cu2ZnSnS4 (CZTS) solar cell is a potential source of low-cost, high efficiency solar electricity [9]. Its constituents are eco-friendly and these have been found much abundant in earth's crust. [10]-[13]. Indeed, CZTS is one of the most prospective materials to be used as solar cell absorber layer, due to its excellent optical properties (the band gap varies from 1.4 to 1.5 eV and the absorption coefficient is higher than 104 cm−1 [14]-[17]

Now in our case, we will use CZTS as absorber layer and different materials such as cadmium sulfide (CdS), Zn(O,S), zinc sulfide (ZnS), zinc selenide (ZnSe), indium sulfide (InS), molybdenum sulfide (MoS2) as buffer layer. The main theme of this simulation is to see the viability of the materials for buffer layers. CZTS thin-film solar cell with the structure of SLG/Mo/CZTS/buffer layer/Al:ZnO was implemented in the SCAPS 3302 environment. The default illumination spectrum and operation temperature were set to the global AM1.5 standard and 300 K, respectively.

II. Device Modeling

The modeling calculations discussed in the following section is done by the software named Solar Cells Capacitance Simulator (SCAPS). SCAPS is a Solar Cell simulation software which was developed under Professor Marc Burgelman in the Department of electronics and information system at University of Ghent, Belgium [18]-[20].

The CZTS structure was made up of a p-type CZTS absorber layer, the buffer layer and n-type Al:ZnO. Molybdenum was used as a back contact and the entire structure was placed on a substrate of Soda Lime Glass. For buffer layer, ZnS is used, but the other materials- CdS, Zn(O, S), ZnSe, InS & MoS2 was used for simulation.

Here CZTS solar cell with the structure of CZTS/buffer layer/Al:ZnO was implemented in the SCAPS 3302. The basic input parameters used in the simulation were adopted from different literatures, theories and some of them were from reasonable estimates in Table I and Table II. The default illumination spectrum and operation temperature were set to the global AM1.5 standard and 300 K, respectively.

III. Results

The performance characteristics of our solar cell models are summarized in Table II. The corresponding J-V curves are shown in Fig. 2-5 respectively. In our simulation Zn(O,S) buffer layer produced the highest efficiency which is 10.28%. It is to be noted that the performances of CdS and Zn(O,S) buffer layers were almost identical CdS fell behind Zn(O,S) only by 0.02% (actual efficiency is 10.26%). Also ZnS showed promising results with good electrical parameters and an efficiency of 9.82%. However the other three materials (ZnSe, InS, MoSe2) showed poor results. ZnSe had a poor energy conversion efficiency of only 1.58%, while the

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Mo|CZTS|InS|Al:ZnO structures failed to converge, that means these buffer layers (InS, MoSe2) are not viable for our model and they will not produce any energy when put under sunlight.

TABLE I: PARAMETERS USED IN THE SIMULATION (1)

Parameters	**CZTS** [21] [22] [23]	**CdS**	**Zn(O,S)** [24] [25] [23]	**ZnS** [9]
Thickness (nm)	2000	50	50	60
Bandgap (eV)	1.5	2.4	2.7	3.5
Electron affinity (eV)	4.5	4.5	4.3	4.5
Dielectric permittivity (relative)	6.5	10	10	10
CB effective density of states ($1/cm^3$)	$2.07*10^{18}$	$2.0*10^{18}$	$2.2*10^{18}$	$1.5*10^{18}$
VB effective density of states ($1/cm^3$)	$8.85*10^{18}$	$1.5*10^{19}$	$1.8*10^{19}$	$1.8*10^{18}$
Electron mobility (cm^2/Vs)	26	50	100	50
Hole Mobility (cm^2/Vs)	10	20	25	20
Shallow uniform donor density, N_D ($1/cm^3$)	0	$1*10^{17}$	$1*10^{17}$	0
Shallow uniform acceptor density, N_A ($1/cm^3$)	$1*10^{16}$	0	0	$1*10^{17}$

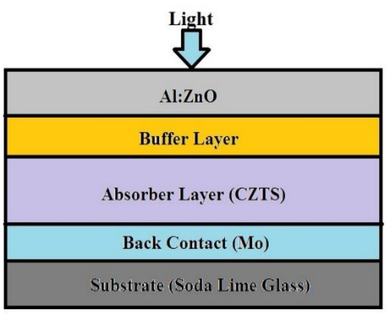

Fig. 1. Structure of a CZTS solar cell.

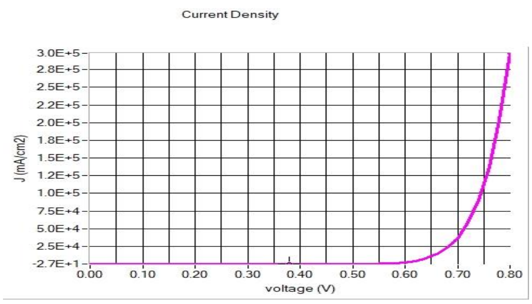

Fig. 2. Light characteristic curve (J vs V) of simulation with CdS buffer layer.

TABLE II: PARAMETERS USED IN THE SIMULATION (2)

Parameters	**ZnSe** [9]	**InS** [9]	**MoS_2** [26]	**Al:ZnO** [27] [28]
Thickness (nm)	80	50	40	200
Bandgap (eV)	2.9	2.8	1.29	3.4
Electron affinity (eV)	4.09	4.7	4.2	4.6
Dielectric permittivity (relative)	10	13.5	4	9
CB effective density of states ($1/cm^3$)	$1.5*10^{18}$	$1.8*10^{19}$	$7.5*10^{17}$	$4*10^{18}$
VB effective density of states ($1/cm^3$)	$1.8*10^{18}$	$4*10^{13}$	$1.8*10^{18}$	$9*10^{18}$
Electron mobility (cm^2/Vs)	50	400	100	100
Hole Mobility (cm^2/Vs)	20	210	150	31
Shallow uniform donor density, N_D ($1/cm^3$)	0	10	0	$1*10^{20}$
Shallow uniform acceptor density, N_A ($1/cm^3$)	$5.5*10^{7}$	$1*10^{18}$	$1*10^{21}$	0

TABLE III: SUMMARY OF PERFORMANCE CHARACTERISTICS OF THE SOLAR CELL

Buffer Layer	**V_{oc}** (volt)	**J_{sc}** (mA/cm^2)	**FF** (%)	**Efficiency** (%)
CdS	0.4804	27.1972	78.53	10.26
Zn(O,S)	0.4803	27.2320	78.57	10.28
ZnS	0.4808	26.8472	76.22	9.82
ZnSe	0.6220	22.1889	11.41	1.58
InS	-	-	-	-
MoS_2	-	-	-	-

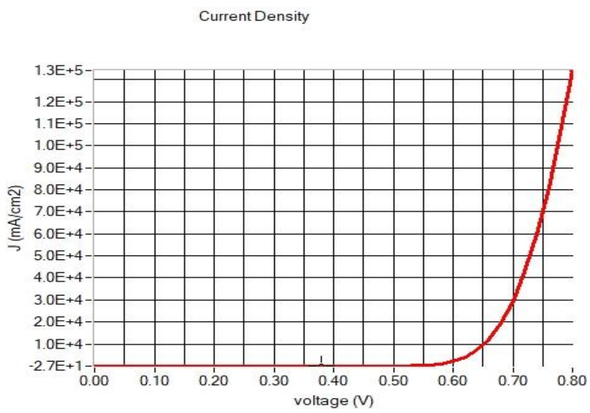

Fig. 3. Light characteristic curve (J vs V) of simulation with Zn(O,S) buffer layer.

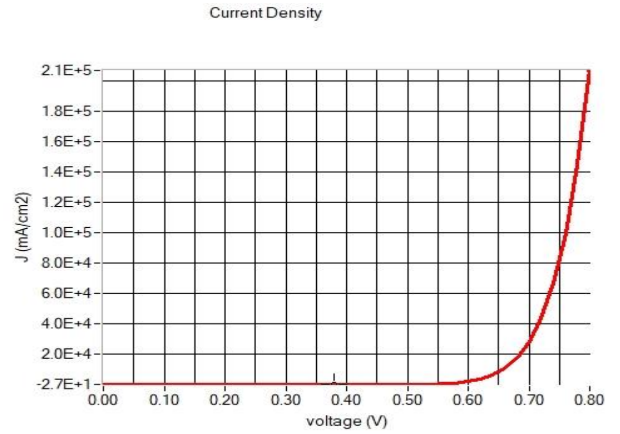

Fig. 4. Light characteristic curve (J vs V) of simulation with ZnS buffer layer.

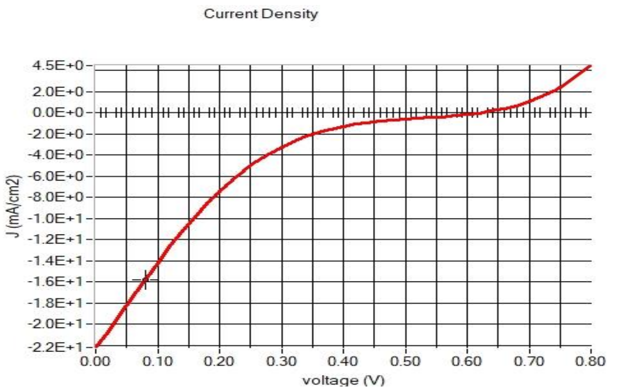

Fig. 5. Light characteristic curve (J vs V) of simulation with ZnSe buffer layer.

IV. Conclusion

From the simulation it can be concluded that different materials can be successfully used with CZTS as buffer layer to implement a solar cell. Especially Zn(O,S) and ZnS showed promising results and hence can be used as an alternative to CdS, which causes serious environmental problem. The Zinc based compounds are abundant, cheap and environment friendly so they are perfect for mass production. One of the major challenges that remain is the comparatively low efficiency of CZTS based solar cells. There is much room for development. Cell models can be further optimized, different materials can be used. Much more improvement in efficiency can be expected from researches being conducted in this field.

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