Performance improvement of CZTS-based solar cells with In2S3 and ZnO dielectric layer as window layer and comparison with CdS layer using SCAPS-1D

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Received: 16-04-2023 Accepted: 28-05-2023 Published: 01-06-2023

Abstract

In the present work, we simulate the i-ZnO/In2S3/p-CZTS/Mo structure based on copper-zinc-tin-sulfur (CZTS). CZTS has become a candidate material for new photovoltaic solar cell due to its excellent properties Where we found that In2S3 is an excellent candidate for the replacement of the CdS dielectric layer in CZTS solar cells. Non-toxic, it has been shown to be a suitable surface composition adaptation for the replacement of the CdS dielectric layer by In2S3. To obtain an interface quality with CZTS layer that makes it possible to control the phenomenon of fault propagation of this interface. SCAPS-1Dsoftware used for simulation CZTS/In2S3/ZnO Thin-film solar cells where the main parts are p-CZTS absorber layer and n-In2S3 insulating layer.

Keywords: Buffer layer, Solar cells , SCAPS-1D, CZTS, ZnO, In2S3, CdS, Simulation, Thin films.

Tob Regul Sci. ™ 2023;9(1): 2487-2494
DOI: doi.org/10.18001/TRS.9.1.170

1. Introduction

In the field of renewable energy, solar cells are used in various terrestrial and space applications. To manufacture cost-effective, high-efficiency and various solar cells, several materials including Si , CdTe , CIGS and organic materials have been considered by many researchers as an absorbent layer for the manufacture of solar cells [1,2]. The renewable energy sector continues to generate great interest in the minds of researchers in recent years. One alternative is thin film solar cells because they consume less material. For example, CdTe relies on expensive and rare elements (such as indium, gallium, and tellur) and toxic materials such as cadmium [3]. CZTS has drawn the attention of researchers over the past years [4]. CZTS is a favored quaternary semiconductor material, because it is made of current and non-toxic elements that are abundant in the Earth. It shows excellent photovoltaic properties such as an absorption coefficient above 10^4 cm^{-1} and a remarkable direct optical bandgap (1.4–1.6 eV) [5]. CdS is used as the standard dielectric layer with a power conversion efficiency of 15.04%. For CZTS, , it has a parasitic absorption in the range of 300–1000 nm, which reduces the efficiency of the device [6]. Indium ternary sulfide (In2S3) a good material to replace cadmium sulfide (CdS) as a dielectric layer in CZTS-based solar cells, is a direct wide band gap compound with a band gap energy of ~2.8 eV and is non-toxic.

2. Numerical Simulation

Figure 1 shows the structure of a solar cell where CZTS is a p-type absorber layer layer, In2S3 as n-type insulating layer SCAPS-1D was used to monitor the effect of difference in carrier concentration and thickness of the CZTS, In2S3 dielectric layer on the performance of the CZTS-based solar cell. Solar cells. In the AM1.5 solar spectrum, where P0 = 100 mW/cm2 and T = 300K. Solar cell performance parameters such as open circuit voltage (Voc), short circuit current density (Jsc), Filling factor (FF) and efficiency (η) were calculated.

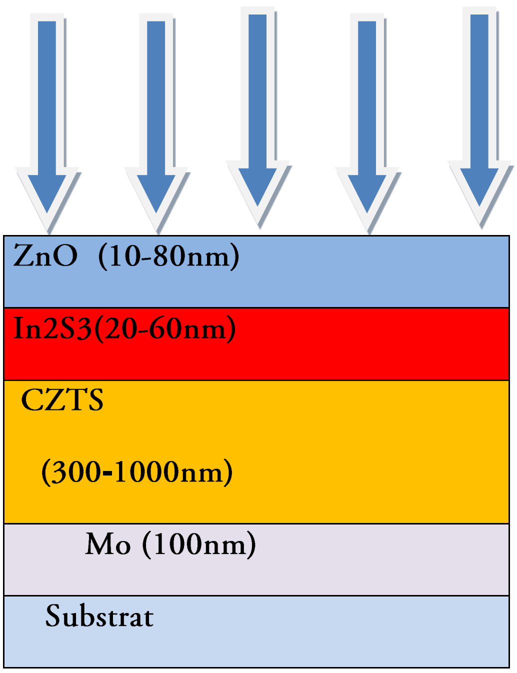

Fig.1. Structure of a CZTS thin film solar cell

The physical parameters used in the study are summarized in Table 1

Table 1. The physical parameters of layer [11,12,13]

Parameter	ZnO	CdS	In_2S_3	CZTS	Mo
Thickness (nm)	10-80	5-50	20-40	300-1000	100
Band gap (eV)	3.30	2.4	2.8	1.4	1.6
Electron affinity (eV)	4.35	4.0	4.5-4.6	4.5	4.177
Dielectric permittivity	9	10	13.5	10	13.6
CB effective density of states (cm^{-3})	2.2 E+18	2.2 E+18	2.2 E+17	2.2 E+18	2.2 E+18
VB effective density of states (cm^{-3})	1.8 E+19	1.8 E+19	1.8 E+19	1.8 E+19	1.8 E+19
Electron thermal velocity (cms^{-1})	1 E+7	1 E+7	1 E+7	1 E+7	1 E+7
Hole thermal velocity (cm^{-1})	1 E+7	1 E+7	1 E+7	1 E+7	1 E+7
Electron mobility (cm^{-1})	25	25	50	20	1 E+2
Hole mobility (cm^2/Vs)	1 E+2	1 E+2	20	1 E+2	25
Shallow uniform donor density, ND (cm^{-3})	1 E+18	1 E+18	1 E+18	0	0
Shallow uniform acceptor density, NA (cm^{-3})	0	0	0	1 E+16	1 E+16

3. Resultsand discussion

3.1. Study In2S3 layer as alternative to CdS layer

In this study, simulations were firstly performed for CZTS/In2S3/ZnO thin-cell solar films, their layering properties are shown in Table 2

Table 2. Properties of different layer CZTS, In2S3 and ZnO

ZnO		**In2S3**		**CZTS**	
Nd (cm^{-1})	**X(mn)**	**Nd** (cm^{-1})	**X(mn)**	**Na** (cm^{-1})	**X(mn)**

10^{18}	10	10^{17}	40	10^{16}	1000

The properties CZTS/In2S3/ZnO solar cell are shown in the Table 3

Table 3. Properties of reference cellCZTS/ In2S3/ZnO

1. Voc	2. Jsc(mA/cm2)	3. FF(%)	4. η(%)
5. 0.7994	6. 30.606198	7. 73.94	8. 18.07

According to Table 3, the reference cell efficiency, estimated at 18.07%, exceeds the cell return value CZTS/ In2S3 recorded in references [8].So in theory we can replace the CdS layer with a In2S3 layer.

3.2. Effect of carrier concentration and thickness of CZTS, In2S3 and fixed concentration and thickness of ZnO 10^{18}(cm^{-1}) and 10 nm

3.2.1. Effect of absorber layer (CZTS) thickness on efficiency

Initially, thickness of the CZTS absorber (Xabsorber) was varied and gap energy is 1.4eV. Figure 3 represents J-V curves of CZTS solar cell and the variations of the solar cell characteristic parameters absorber versus a thickness.

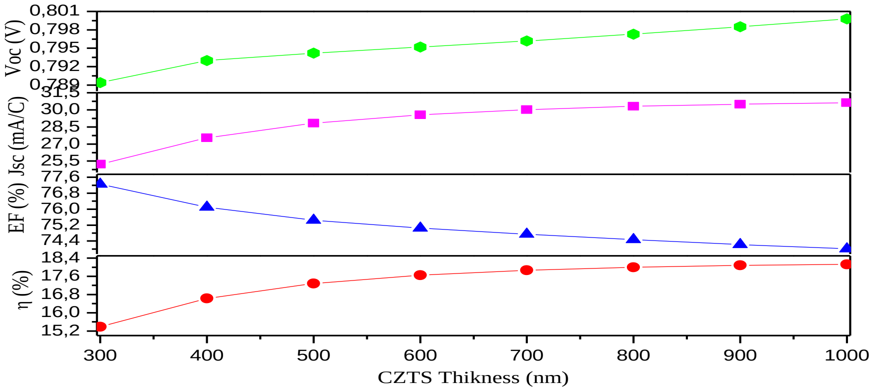

Fig. 3. (a) J-V curves of CZTS solar cell, (b) Performance variation due to variable thickness of the CZTS absorber layer.

3.2.2. Effect of carrier concentration of CdS Absorber Layer

The CdS absorber layer doping concentration is changed from 1×10^{13} to 1×10^{18} cm-3. CdS doping anisotropy: by setting the thickness to 10 nmet, the defect density Nt = 6.1016 cm-3 and the gap Eg = 2.4 EV .ZnO thickness is 20nm and CZTS thickness is 1000nm . Figure 4 shows the absorber layer doping effect on the electrical parameters (Jsc, Voc, FF, and efficiency).

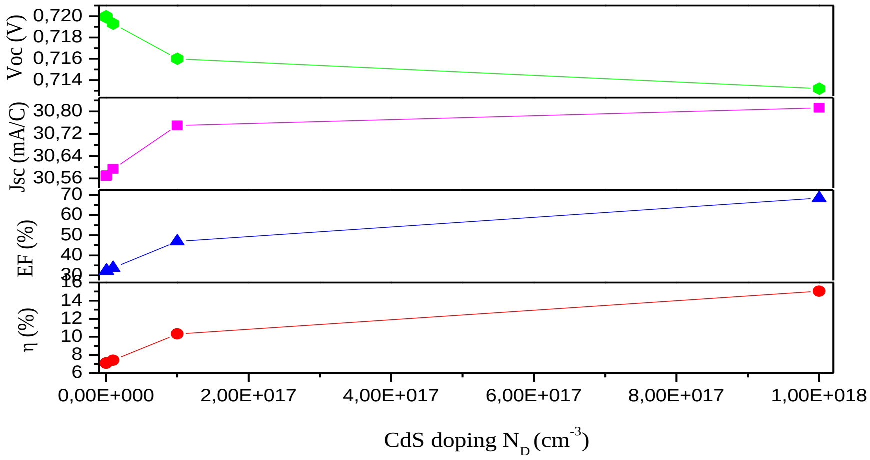

Fig.4. Effect of carrier concentration of CdS

From Fig. 4, the efficiency increases with increasing doping of the CdS absorber Layer until it reaches a yield value of about 15.04% at concentration (10^{18} cm^{-3}) Benefit of increasing doping The focus is an increase in electrical conductivity, from which we conclude that the efficiency variance is constant. Therefore, we consider the value of the yield obtained as an ideal value. [8]

3.2.3. Effect of carrier concentration of In2S3 buffer layer

To study the effect of the sequestrant In2S3 carrier concentration on the solar cell, simulations were performed .On the structure shown in Fig. 5, the thickness of the In2S3 dielectric layer should be maintained about 40 nm to reduce the absorption loss in the dielectric layer. It is clearly seen from Figure 5 during the control or reduction of the doping concentration The absorbent layer is at an optimal value of 10^{17} cm^{-3} [8]. that constant *V*ocbe with increasing carrier In2S3 concentration leads to elevated Jsc and FF, This led to better efficiency on the solar cell .There is a direct proportion between them.

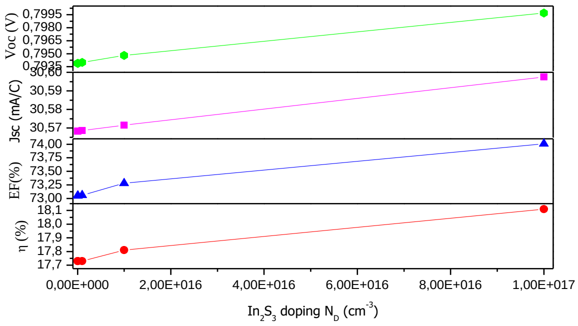

Fig.5. Effect of carrier concentration of In2S3 layer

3.2.4. Effect of In2S3 buffer thickness

The thickness of the In2S3 layer was changed from 20 nm to 60 nm to study the effect of the thickness of the insulating layer on cell performance (Fig. 6). From Fig. 6 it is seen that the constant *V*ocbe with increasing thickness of In2S3. Lower Jsc and FF lead to lower solar cell efficiency, and vice versa. But over 30 nm the solar fill factor, except for *V*oct which is approximately constant. This is explained by the very abundant absorption of photons in this layer. Absorption in the dielectric layer reduces the incident number of photons having energy hv > Eg (dielectric layer) [9,8]

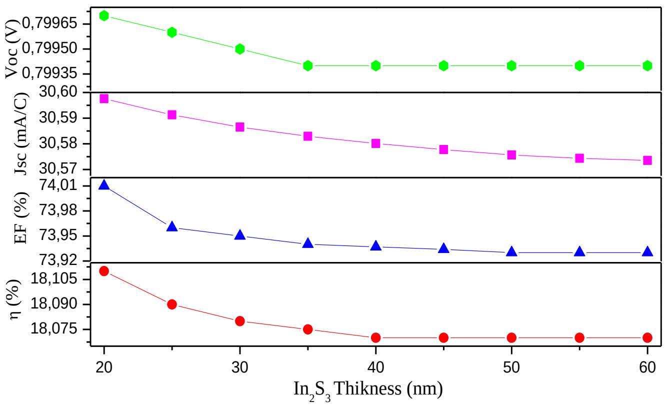

Fig. 6. Effect of thickness of In2S3 layer on *V*oc, Jsc, fills factor and efficiency

Conclusions

In this study, we performed numerical simulation using the SCAPS-1D package for observation Solar cell performance by varying the optimal carrier thickness and concentration in the CZTS solar cell shows that the optimal thickness and band gap of the absorber layer are 1000 nm and

1.4 V, respectively with the In2S3 dielectric layer. Investigation. We find that the optimal carrier concentration in the CZTS adsorption layer is 10^{16} cm^3, 10^{17} cm^3 in the In2S3 dielectric layer and 10^{18} cm^3 in the ZnO window layer. By simulating all the parameters we found that the solar cell with In2S3 has the highest Efficiency compared with a layer of insulating and toxic CdS, where the efficiency of In2S3 was (efficiency = 18.07%).

Acknowledgments

The authors gratefully acknowledge to Dr. Marc Burgelman, University of Gent, Belgium, for providing the SCAPS simulation software.

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