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Modeling and simulation of CZTS based solar cells with ZnS buffer layer and ZnO:F as a window layer using SCAPS-1D

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ZnS is an excellent candidate for the substitution of the CdS buffer layer inCZTS based solar cells, is nontoxic and is relatively less costly.It has been shown that a surface composition adaptation is favorable for the replacement of the buffer layer CdS by ZnS so as to obtain an interface quality with the CZTS layer that makes it possible to control the diffusion phenomenon of faults to this interface. SCAPS-1Dsoftware is used to simulate CZTS/ZnS/ZnO:F thin-film solar cell where the key parts are p-CZTS absorber layer and n-ZnS buffer layer.

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Keywords: Buffer layer, CZTS, SCAPS-1D, ZnO:F, ZnS.

1. Introduction

In the field of renewable energy, Solar cells are used in various terrestrial and space applications. For the fabrication of solar cell with a cost-effective and highly efficient, different materials such as Si, CdTe, CIGS, and organic materials have been considered by many researchers as an absorber layer for the fabrication of solar cell [1,2]. But due to the toxicity of cadmium and selenium, and less availability of tellurium and indium, CZTS material has achieved great attraction among the researchers during last couple of years [3,4].

CZTS is a quaternary semiconductor with non-toxic earth-abundant constituent material. It exhibits excellent photovoltaic properties such as absorption coefficient above$10^4 cm^{-1}$and appreciable direct optical band gap (1–1.5 eV) [5-8].

CdS is used as a standard buffer layer which has, a power conversion efficiency of 12.6% for CZTS [9,10], having parasitic absorption in the 350–550 nm range, which decrease the efficiency of the device[11,12]. Zinc sulfide (ZnS), is a good material to replace the cadmium sulfide(CdS) as the buffer layer in CZTS based solar cells, is a direct wide band gap compound with a band gap energy of ∼3.8 eV and non-toxic.

2. Numerical Simulation

Figure 1 shows the structure of the solar cell where CZTS is the p-type absorber layer layer, ZnS as n-type buffer layer and ZnO:F as a window layer. Fluorine appears as one of the best candidate to dope the ZnO and high performances of ZnO:F have already been demonstrated [13].

SCAPS-1D has been used to observe the effect of variation in carrier concentration and thickness of CZTS, ZnS buffer layer and ZnO:F window layer into the performance of the CZTS solar cell. in the AM1.5 solar spectrum, with P_0 =100 mW/cm^2 and T=300K. Solar cell performance parameters such as open circuit voltage (V_{oc}), short circuit current density (J_{sc}), fill factor (FF) and efficiency (η) have been calculated

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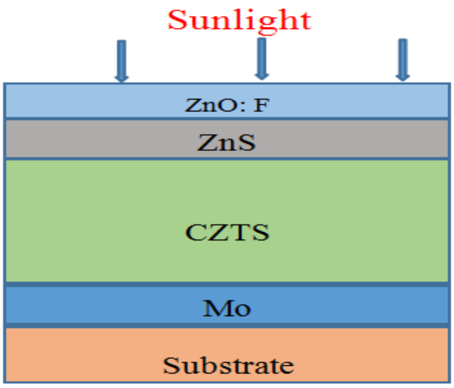

Fig.1. Structure of a CZTS thin film solar cell.

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

Table 1. The physical parameters of layer [14-16].

Parameter	CZTS	ZnS	ZnO : F
Band gap (eV)	1.5	3.7	3.2
Electron affinity (eV)	4.5	4.5	4.5
Dielectric permittivity	10	9	10
CB effective density of states (cm^{-3})	2.2×10^{18}	2.2×10^{18}	4×10^{18}
VB effective density of states (cm^{-3})	1.8×10^{19}	1.8×10^{19}	4×10^{19}
Electron thermal velocity (cms^{-1})	1×10^{7}	1×10^{7}	1×10^{7}
Hole thermal velocity (cm^{-1})	1×10^{7}	1×10^{7}	1×10^{7}
Electron mobility (cm^2/V_s)	100	100	100
Hole mobility (cm^2/V_s)	25	25	25
Shallow uniform donor density, N_D (cm^{-3})	1×10^{1}	Varying	Varying
Shallow uniform acceptor density, N_A (cm^{-3})	Varying	0	0

3. Resultsand discussion

3.1. Study ZnS layer as alternative to CdS layer

In this study, first the simulations have been done for CZTS/ZnS/ZnO:F thin-film solar cell, its layers properties is shown in the table2.

Table 2.Properties of different layer CZTS, ZnS and ZnO:F.

ZnO:F		**ZnS**		**CZTS**	
$N_d(cm^{-1})$	**X(nm)**	**$N_d(cm^{-1})$**	**X(nm)**	**$N_a(cm^{-1})$**	**X(nm)**
10^{17}	**10**	**10^{17}**	**50**	**10^{18}**	**3000**

The J-V characteristics for CZTS solar cell have been simulated in figure 2.

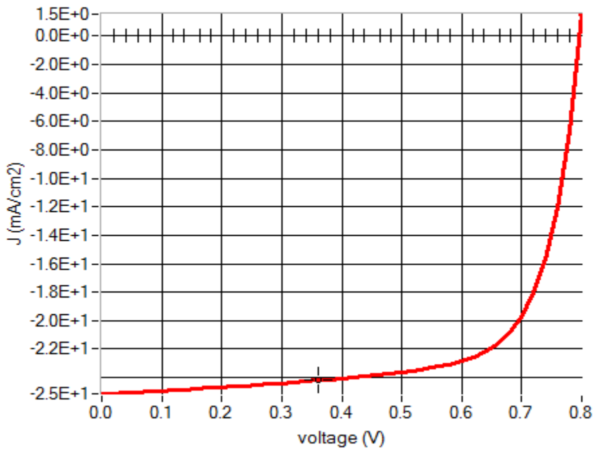

Fig.2. J-V curves of CZTS/ZnS/ZnO:F solar cell.

The properties CZTS/ZnS/ZnO:F solar cell are shown in the Table 3.

Table 3.Properties of reference cellCZTS/ZnS/ZnO:F.

V_{oc}	J_{sc}(mA/cm^2)	FF(%)	η(%)
0.7967	25.145355	71.30	14.28

According to Table 3, the reference cell efficiency, estimated at 14.28%, exceeds the cell return value CZTS/CdS recorded in references [16,17].So in theory we can replace the CdS layer with a ZnS layer.

3.2. Effect of carrier concentration and thickness of CZTS, ZnS and ZnO:F

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

Initially, thickness of the CZTS absorber ($X_{absorber}$) was varied and gap energy is 1.5eV.Figure 3 (a) and Figure 3 (b) represents J-V curves of CZTS solar cell and the variations of the solar cell characteristic parameters absorber versus a thickness.

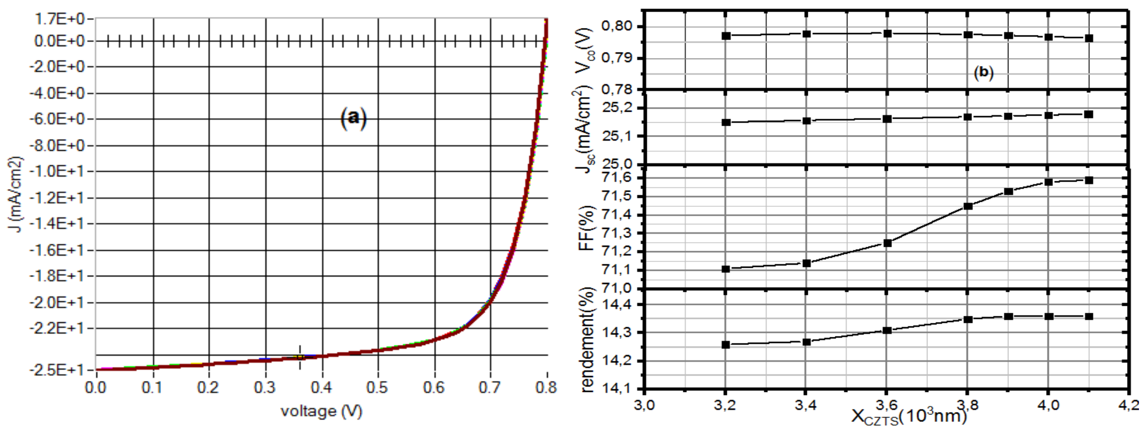

Fig. 3. (a) J-V curves of CZTS solar cell, (b) Performance variation due to variable thickness of the CZTS absorber layer.

Figure 3 (a) and Figure 3 (b) shown that the solar cell efficiency (η) increases with the increase of the CZTS absorber thickness, but over 3.9 μm, the efficiency variation seems to be constant until the maximum value is 14.36%. This value so we consider it an ideal value. This may mainly because that more photons with longer wavelength can be absorbed by the absorber if the absorber layer is thicker, and thus the more electron-ho pairs are generated [16,18,19,20].

3.2.2. Effect of carrier concentration of CZTS Absorber Layer

The CZTSabsorber layer doping concentration is changed from 1×10^{15} to 8×10^{16} cm^{-3}.The band gap of the absorber is also kept constant to 1.5 eV. Figure 4 shows the absorber layer doping effect on the electrical parameters (J_{sc}, V_{oc}, FF, and efficiency).

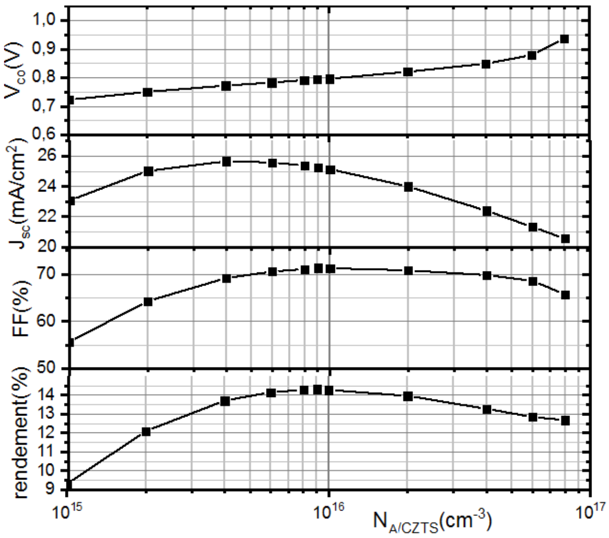

Fig.4. Effect of carrier concentration of CZTS.

From the figure 4, the efficiency increases with increasing doping of the CZTS absorber layer from 9.30 % (10^{15} cm^{-3}) to 14.32 % (9×10^{15} cm^{-3}), The benefit of an increase in doping concentration is an increase in the electrical conductivity [18], but the doping concentration or defects in semiconductors it often exceeds a certain threshold and becomes a loss factor. The efficiency variation seems to be constant. This value so we consider it an ideal value.

3.2.3. Effect of carrier concentration of ZnSbuffer layer

To study the effect of carrier concentration of ZnS buffer on the solar cell, simulations has been done on the structure shown in Figure 5, the thickness of the ZnS buffer layer should be kept around 50 nm to reduce the absorption loss in the buffer layer.

It is clearly observed From Figure 5 that the V_{oc}be constant with the increase of the carrier concentration of ZnS.The decrease of J_{sc} and FF leads to the decrease of the efficiency of the solar cells.

This is a good reason to reduce large carrier concentration values. So, in order to obtain a better Efficiency on the solar cell, it is necessary to control or limit the doping concentration in the absorbent layer [18].

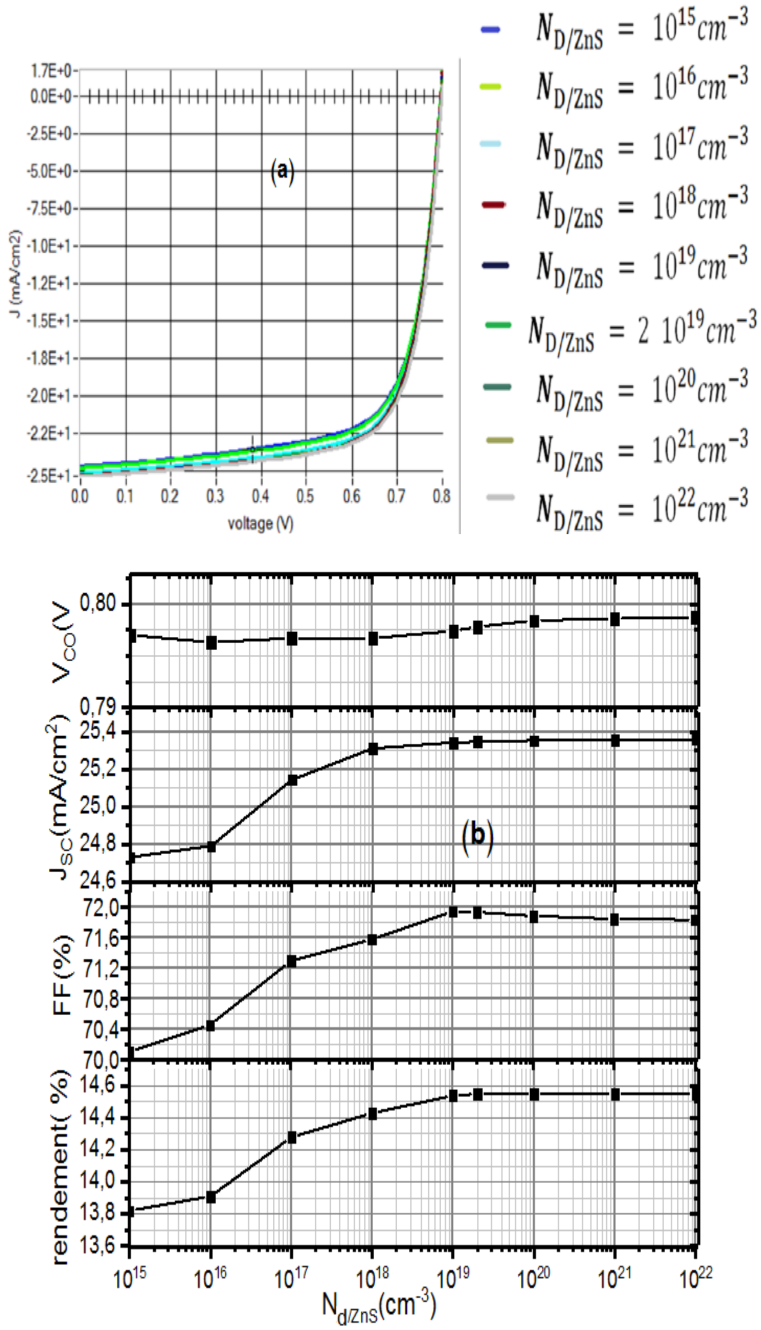

Fig.5. (a) J-V curves of CZTS solar cell, (b)Effect of carrier concentration of ZnS layer.

3.2.4. Effect of ZnSbuffer thickness

The thickness of the ZnS layer is changed from 2 nm to 50 nm to study the influence of buffer layer thickness in the cell performance (Figure 6).

From Figure 6, it is clearly observed that the V_{oc}be constant with the increase of thickness of ZnS. The decrease of J_{sc} and FF leads to the decrease of the efficiency of the solar cells, but over 25 nm the solar Fill Factor, except for V_{oc}that is almost constant. This is explained by a significant absorption of photons in this layer. The absorption in the buffer layer reduces the number of photons incidents which have an energy hv> Eg (buffer layer) [17,18].

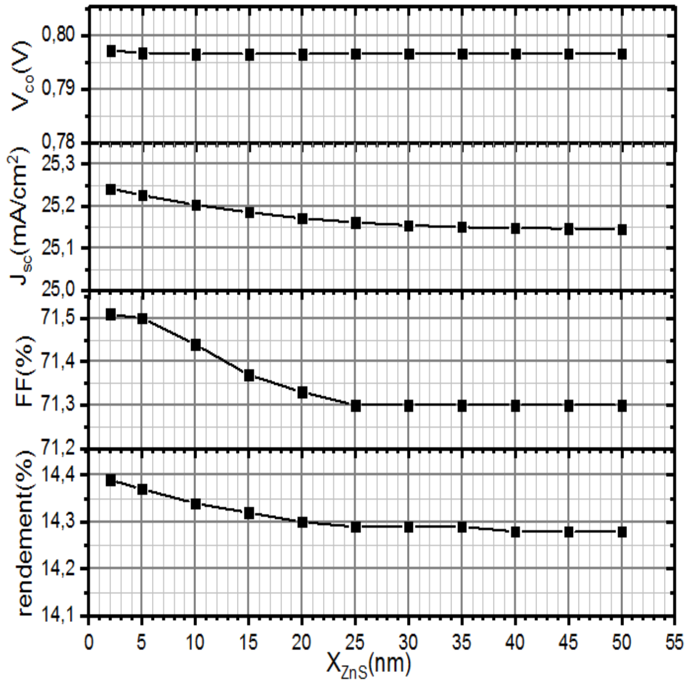

Fig. 6. Effect of thickness of ZnS layer on V_{oc}, J_{sc}, fills factor and efficiency.

3.2.5.Effect of carrier concentration of ZnO:Fwindow layer

To study the effect of carrier concentration of ZnO:F window on the solar cell, simulations have been done on the structure shown in Figure 7.

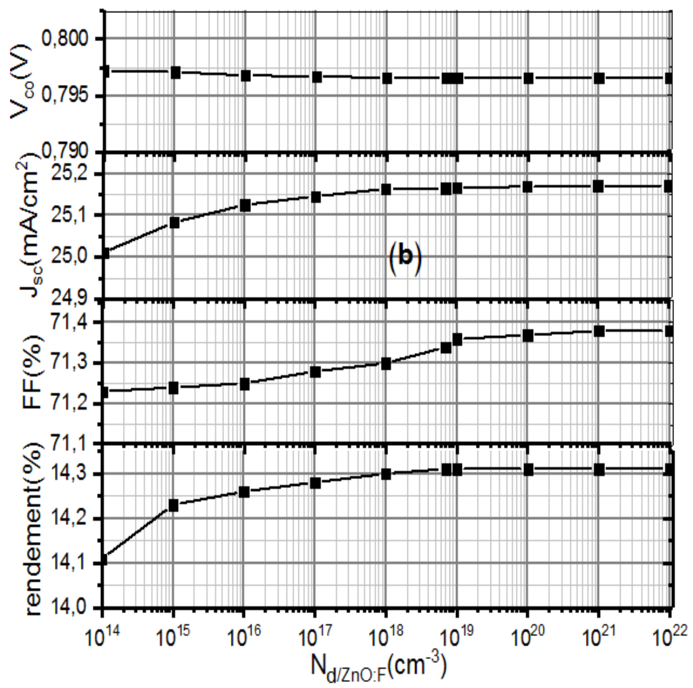

Fig.7. Effect of carrier concentration of ZnO:Fwindow layer.

From Figure 7, it is clearly observed that the V_{oc}be constant with the increase of the carrier concentration of ZnO:F window layer. The decrease of J_{sc} and FF leads to the decrease of the efficiency of the solar cells. Increasing the thickness of this layer increases the number of photons absorbed at their level, so the photons absorbed in this layer are converted to thermal energy and decrease the permeability of the photons,This results in a decrease in the value of current and efficiency [17].

3.2.6.Effect of ZnO:F window layer thickness

The thickness of the window layer is changed from 0 to maximum 200 nm, and simulation results are illustrated in Figure 8.It can be seen that, the increase of buffer layer thickness decreases J_{sc}, FF and Efficiency, but V_{oc} be constant.

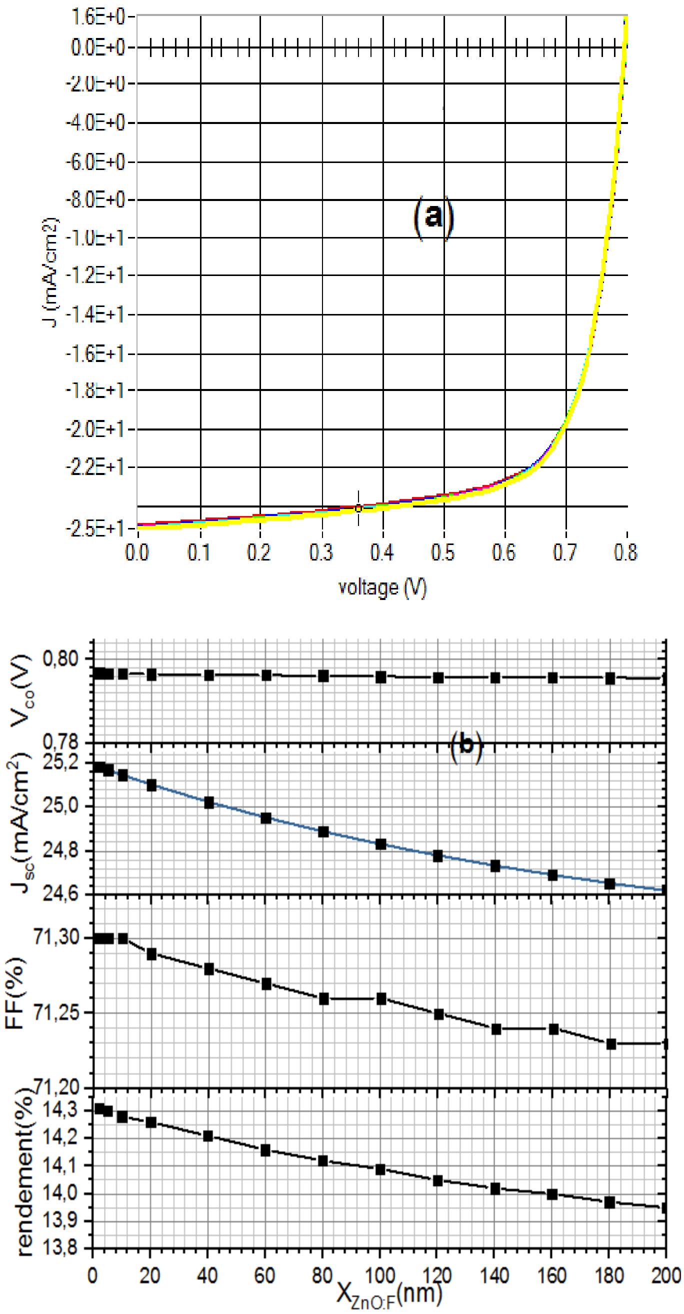

Fig.8. (a) J-V curves of CZTS solar cell,(b) Effect of thickness of ZnO:F window layer.

From Figure 8 (a) and (b), the V_{oc}be constant with the increase of thickness of ZnO:F window layer. The decrease of J_{sc} and FF leads to the decrease of the efficiency of the solar cells, but over 25 nm the solar Fill Factor, V_{oc}variation seems to be constant. The first contact between photons and the solar cell is the window layer ZnO:F that can reflect It absorbs some of the photons coming to the front side of the cell. Increasing the thickness of this layer increases The number of photons absorbed at each level (the photons absorbed in this layer are converted to thermal energy), With this, the photo transmittance is reduced to the buffer and absorbent layers that occur in the photoelectric process and decreases Couples generate an electron-hole, which results in a decrease in the current and return value. [16,17].

Conclusions

The performance measurements in the CZTS solar cell with a ZnS buffer layer have been investigated. We find that the optimum carrier concentration in the CZTS absorber layer is 10^{16} cm^{-3}, 10^{17} cm^{-3} in the ZnS buffer layer and $7x10^{18}$ cm^{-3} in the ZnO:F window layer.

Simulating all the parameters we have found that the solar cell with ZnS has the highest efficiency (efficiency=14.61%,FF=71.94%, J_{sc}=25.40mA/cm^2 & V_{oc}= 0.79V) among all other considered buffer layers.

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