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Effect of $Cd_{1-x}Zn_xS$ Window Layer Incorporation in CdTe Solar Cell by Numerical Simulation

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Abstract— **CdTe is a very potential binary semiconductor material for solar photovoltaic application due to its superior optoelectronic properties. The overall performances of incorporating $Cd_{1-x}Zn_xS$ window layer in lieu of CdS layer in CdTe solar cell were investigated by SCAPS-1D simulator. The $Cd_{1-x}Zn_xS$ is an alloy of CdS and ZnS which increase band gap of window layer from 2.42 eV to 3.7 eV as a function of x (from x=0 to 1). The spectral response of the design $Cd_{1-x}Zn_xS$/CdTe cell improves in blue region which implies the big improvement of short circuit current density J_{sc}. In addition, in the traditional back contact of CdTe cell a small positive conduction band (ΔEc <0.3 eV) offset is necessary to reduce the forward current J_0 as well as the recombination losses at the back contact. To achieve this goal a highly doped ZnTe:Cu extra layer was used as an electron reflector (ER) above back contact. Furthermore, this ER interface allows electron tunnelling by reducing the barrier height of the valence band which in turn leads to an improvement of open circuit voltage and fill factor. The performance of the proposed cell was examined by varying thickness and doping concentration of transparent conducting oxide (TCO) layer, window layer, absorber layer and finally ER layer. The simulated results of the proposed cell had shown that the open circuit voltage (V_{oc}) overcame the 1-volt barrier of CdTe cell with energy conversion efficiencies of 19.93 %.**

Index Terms—*$Cd_{1-x}Zn_xS$ window layer; CdTe Solar cell; ZnTe:Cu electron reflector; back contact.*

I. INTRODUCTION

CdTe solar cell is a leading low cost and efficient thin-film photovoltaic technology for the deployment in the large terrestrial application. The performance limit of CdTe cell and module reaches over 22% and 18% respectively primarily due to the improvement of the photocurrent enhancement [1]. Further, the manufacturing cost of the PV module reduced to \$0.51/W in 2015 and the cost of energy is around 0.0387 \$ kWh [2-3]. CdS (Eg=2.42 eV) has been considered as a suitable hetero partner of CdTe absorber layer for junction formation but it causes high absorption especially in short wavelength region below 510 nm [4-5]. Therefore, to improve the blue response a very thinner CdS window layer is recommended. Reduced CdS window layer leads pinhole and micro shunt related problem with transparent conducting oxide (TCO) which in turn reduce device V_{oc} and fill factor (FF) [6-8]. An additional high resistivity transparent layer is necessary to overcome shunting which also increase device series resistance and fabrication steps. To improve the device performance of CdTe cell especially in the blue region and to reduce window/absorber interface recombination, researchers investigated different window materials. The $Cd_{1-x}Zn_xS$ film has a tuneable direct band gap of 2.42 eV to 3.7 eV with varying x ratio x=Zn/ (Zn+Cd), from x=0 to 1 [9-11]. Incorporation of $Cd_{1-x}Zn_xS$ film in CdTe cell structure improves J_{sc} and overall efficiency of the cell [12-13]. There are various fabrication methods in which $Cd_{1-x}Zn_xS$ film are deposited such as metal organic chemical vapor deposition (MOCVD) [9], chemical bath deposition (CBD) [11], atmospheric pressure metal organic chemical vapor deposition (AP-MOCVD) [12], RF sputtering [13] and so on. In this paper, the response of incorporation of $Cd_{1-x}Zn_xS$ window layer in CdTe solar cell has been explored by SCAPS-1D simulator.

II. MODELING AND SIMULATION

The typical structure of CdTe solar cell (SnO_2/CdS/CdTe/Cu doped graphite paste) was modified by the different researchers for improving the device performance [4-5, 8].

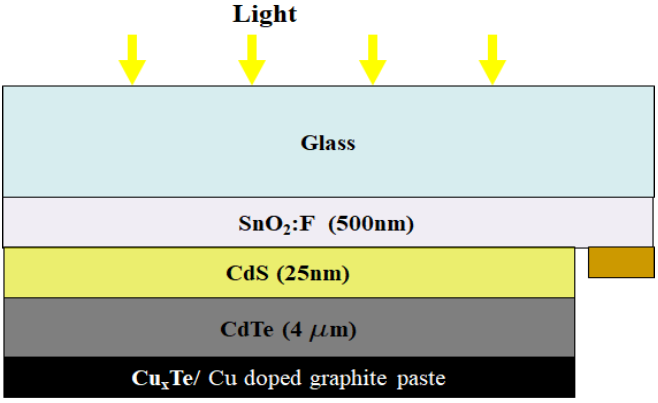

Fig. 1 Base cell structure of CdTe solar cell [14]

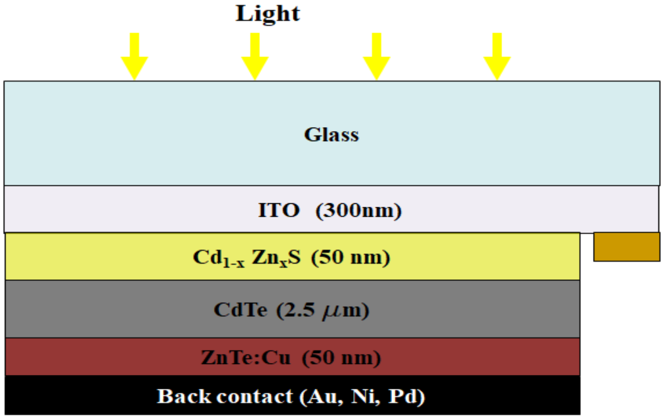

Fig. 2 Modified CdTe solar cell structure

In this paper, the conventional CdTe solar cells modelled by M. Gloeckler has been considered as a base cell whose performance parameters (J_{sc} = 24.6 mA/cm^2, V_{oc} = 0.87 V, FF = 76%, and η = 16.4%) at AM 1.5G and T=300 K conditions

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[14]. The baseline cell model and modified cell structures of CdTe are shown in Fig. 1 and Fig. 2 respectively. In this modified structure, Indium Tin Oxide (ITO) layer is used as a transparent front contact with doping concentration (10^{17} - 10^{19} cm^{-3}) and $Cd_{1-x}Zn_xS$ ternary alloy is used as a window layer with adjustable material properties. Table I presents the material parameters used in this simulation taken from previous work done by the researchers [14-20]. The $Cd_{1-x}Zn_xS$ window layer improves short-circuit current density J_{sc} of the cell. However, the overall performance of the cell is not good enough due to interface recombination in back contact of CdTe solar cell.

TABLE I: MATERIAL PARAMETERS USED IN SIMULATION [14-20]

<table>
<tr><th colspan="5">General Device Properties</th></tr>
<tr><td colspan="2"></td><td>Front</td><td colspan="2">Back</td></tr>
<tr><td colspan="2">φb [Ev]</td><td>φbn =0.1</td><td colspan="2">φbp =0.4</td></tr>
<tr><td colspan="2">Se[cm/s]</td><td>10^7</td><td colspan="2">10^7</td></tr>
<tr><td colspan="2">Sh[cm/s]</td><td>10^7</td><td colspan="2">10^7</td></tr>
<tr><td colspan="2">Reflectivity R_f</td><td>0.1</td><td colspan="2">0.8</td></tr>
<tr><th colspan="5">Layer Properties</th></tr>
<tr><th>Parameters</th><th>ITO</th><th>$Cd_{0.2}Zn_{0.8}S$</th><th>CdTe</th><th>ZnTe</th></tr>
<tr><td>W (nm)</td><td>300</td><td>50</td><td>40000</td><td>50</td></tr>
<tr><td>$\varepsilon/\varepsilon_0$</td><td>9.4</td><td>9</td><td>9.4</td><td>10.3</td></tr>
<tr><td>μc (cm^2/Vs)</td><td>30</td><td>100</td><td>320</td><td>70</td></tr>
<tr><td>μp (cm^2/Vs)</td><td>5</td><td>40</td><td>40</td><td>50</td></tr>
<tr><td>n, p (cm^{-3})</td><td>n:10^{18}</td><td>n:10^{18}</td><td>p:2×10^{14}</td><td>p:7.5×10^{19}</td></tr>
<tr><td>Eg (eV)</td><td>3.72</td><td>3.3</td><td>1.45</td><td>2.25</td></tr>
<tr><td>Nc (cm^{-3})</td><td>4.3×10^{20}</td><td>2.1×10^{18}</td><td>8×10^{17}</td><td>7.5×10^{17}</td></tr>
<tr><td>Nv (cm^{-3})</td><td>4×10^{19}</td><td>1.7×10^{18}</td><td>1.8×1^{19}</td><td>1.5×10^{19}</td></tr>
<tr><td>χ (eV)</td><td>3.6</td><td>4</td><td>4.28</td><td>3.53</td></tr>
</table>

To reduce the interface recombination at the back contact, a stable ohmic back contact is significantly required for achieving higher performance from the CdTe cell. CdTe has high electron affinity ($\chi = 4.5$) and moderate band gap (E_g= $1.45eV$). Hence, a metal with a high work function ($\varphi m \geq 5.9\ eV$) is required to form an ohmic contact but most metals do not have a sufficiently high work function. Thus, CdTe makes a blocking Schottky back contact with barrier height (φb). Metallic interface is calculated using equation (1) and the metal with higher work function as well as their barrier (φb) are shown in Table II [21-22]. In addition, how the barrier height (φb) affects CdTe cell performance parameters J_{sc}, V_{oc} and FF are illustrated in Fig. 2.

$$\varphi b = E_g q + (\chi - \varphi m) \qquad (1)$$

TABLE II METAL WORK FUNCTION WITH BARRIER HEIGHT

Metal	φm	φb
	eV	eV
Al	4.28	1.67
V	4.3	1.65
Cr	4.5	1.45
Sb	4.55	1.4
Mo	4.6	1.35
Cu	4.65	1.3
Ag	4.7	1.25
Te	4.95	1
Au	5.1	0.85
Pd	5.12	0.83
Ni	5.15	0.8
Pt	5.65	0.3

The characteristics equations for evaluating solar cell performance are: Short-circuits current density (J_{sc}), open-circuit voltage (V_{oc}) and fill factor (FF) is denoted by the given equation (2)-(4). In Fig. 3, it is shown that to maximize the efficiency of CdTe solar cell it is necessary to minimize the forward current.

Short-circuits current density (J_{SC}):

$$J_{sc} = J_o\left(e^{\frac{qV}{KT}} - 1\right) - J_L \qquad (2)$$

Open-circuit voltage (V_{OC}):

$$V_{oc} = \frac{qV}{KT}\ln\left(\frac{J_{sc}}{J_o} + 1\right) \qquad (3)$$

Fill factor (FF):

$$FF = \frac{v_{oc} - \ln(v_{oc} + 0.72)}{v_{oc}} \qquad (4)$$

$$\text{Where, } v_{oc} = \frac{V_{oc}}{KT/q}$$

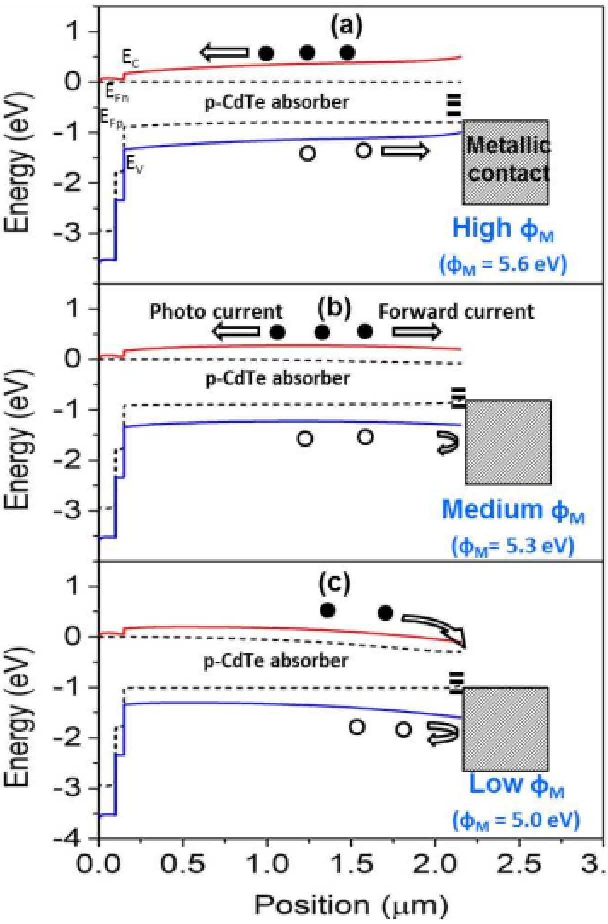

Fig. 3 Band diagrams of CdTe cells with different metal work function [2]

As a consequence, highly doped ZnTe:Cu has been used as an ER layer to reduce the barrier height for the hole and allow tunnelling [23-24]. Further, this ER layer makes a forward conduction offset ($\Delta Ec > 0$) which reduce the forward current as well as improve the overall cell performance.

III. RESULTS AND DISCUSSION

A. Impact of $Cd_{1-x}Zn_xS$ window layer on cell performance

In this simulation the band gap of the $Cd_{1-x}Zn_xS$ alloys is calculated by equation (5) for x=0.8 [12].

$$E_g(x) = E_g(CdS) + [E_g(ZnS) - E_g(CdS) - b]x + bx^2 \qquad (5)$$

Where, E_g (CdS) = 2.42 *eV*, E_g (ZnS) = 3.72 *eV*, and the bowing parameter b = 0.91 *eV*. The impact of $Cd_{0.2}Zn_{0.8}S$ window layer on cell performance has been evaluated numerically and its characteristics are compared with CdS window layer by varying their thickness from 25 nm to 200 nm and doping concentrations from 10^{16} cm^{-3} to 5.1x10^{19} cm^{-3}. The simulated result is presented in Fig. 4.

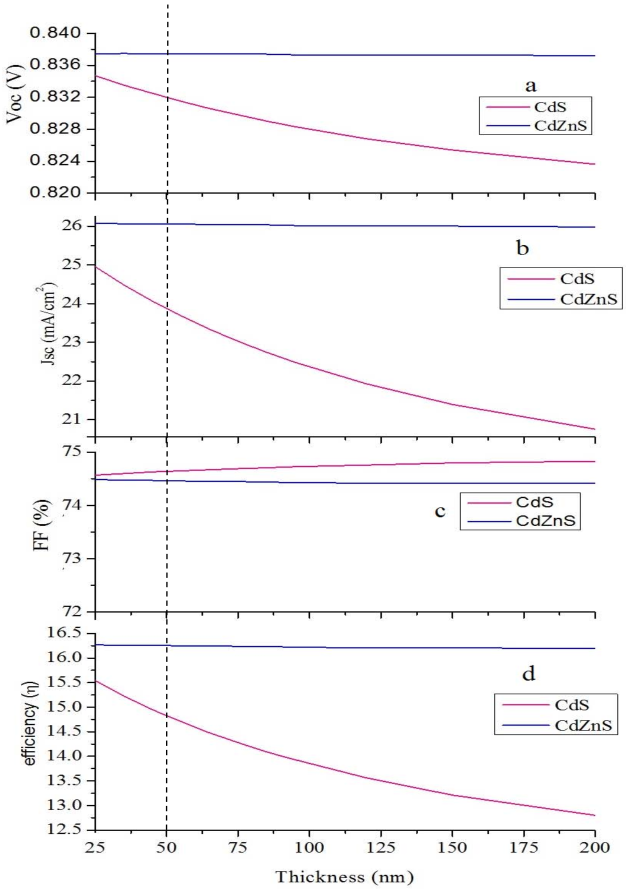

Fig. 4 Effect of window layer thickness variation on: (a) *Voc*, (b) *Jsc* (c) FF and (d) efficiency

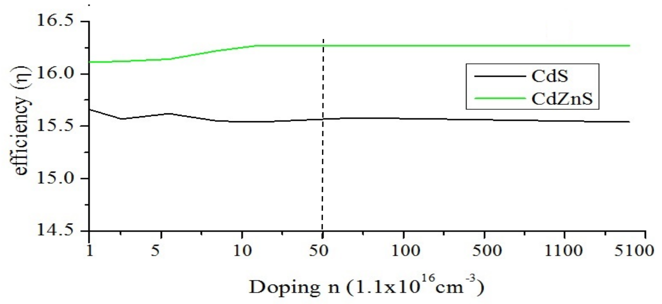

Fig. 5 Effect of window layer doping concentration on overall efficiency

In the case of CdS widow layer, V_{oc} and J_{sc} are highly sensitive with its thickness and both the properties are decreasing whereas the FF shows opposite nature. On the other hand, $Cd_{0.2}Zn_{0.8}S$ alloy shows less sensitivity with its thickness but the overall performance of the base cell is improved as shown in Fig. 4. Further, when the doping concentration of both widow layers changed then it is found that the overall response of $Cd_{0.2}Zn_{0.8}S$ layer much better than CdS as shown in Fig. 5.

B. Effect of CdTe absorber layer on cell performance

The performance of ITO/$Cd_{0.2}Zn_{0.8}S$/CdTe/Au cell is further investigated by changing the CdTe absorber material process parameter and the simulated result is shown in Fig. 6.

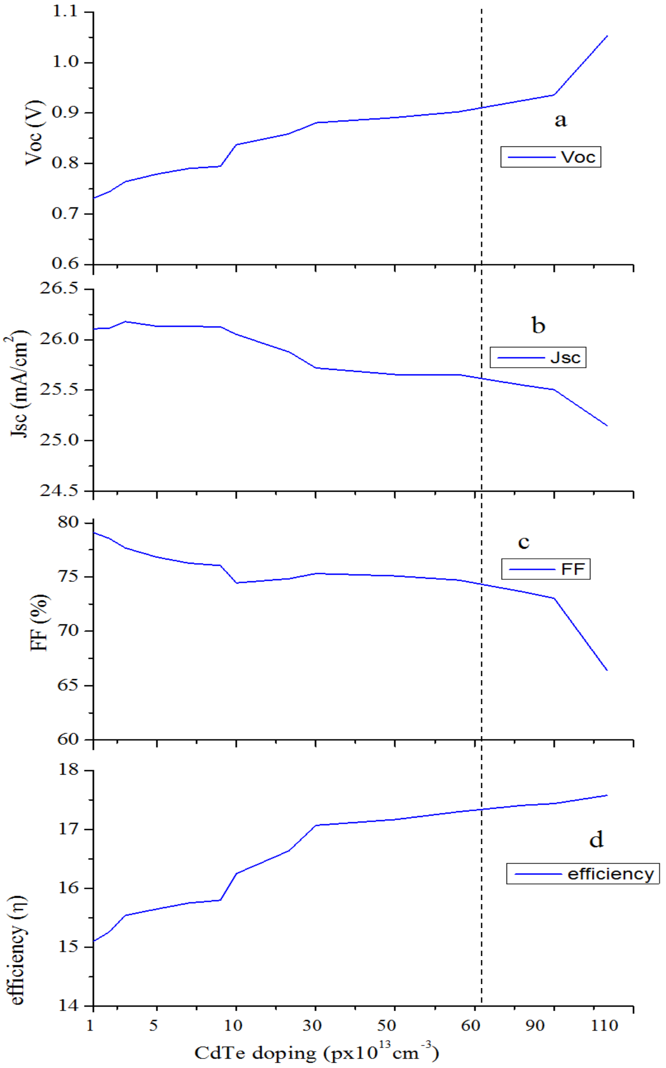

Fig. 6 Effect of CdTe layer doping concentration variation on ITO/Cd0.2Zn0.8S/CdTe cell parameters without ER layer (a) *Voc*, (b) *Jsc* (c) FF and (d) efficiency

Open circuit voltage V_{oc} of CdTe solar cell almost shows linear response with the increase of hole concentration from 1×10^{13} cm^3 to 3×10^{15} cm^3 whereas there is gradual decrement of J_{sc} observed. In addition, the improvement of V_{oc} is neutralized by the dramatic fall of *FF* over 9×10^{14} cm^3 hole concentration. The decrease of J_{sc} might be the causes of interface recombination at back contact which in turn increase the forward current. The optimum efficiency (17.58 %) for ITO/$Cd_{0.2}Zn_{0.8}S$/CdTe/Au cell without ER layer is found at a doping level 1×10^{15} cm^3 where J_{sc}=25.15 mA/cm^2, V_{oc}=1.05 V and FF =66.41. While increasing the thickness of the CdTe absorber layer, it is found that the cell reaches its optimum efficiency limit at 3 μm thickness beyond this any further improvement were not observed.

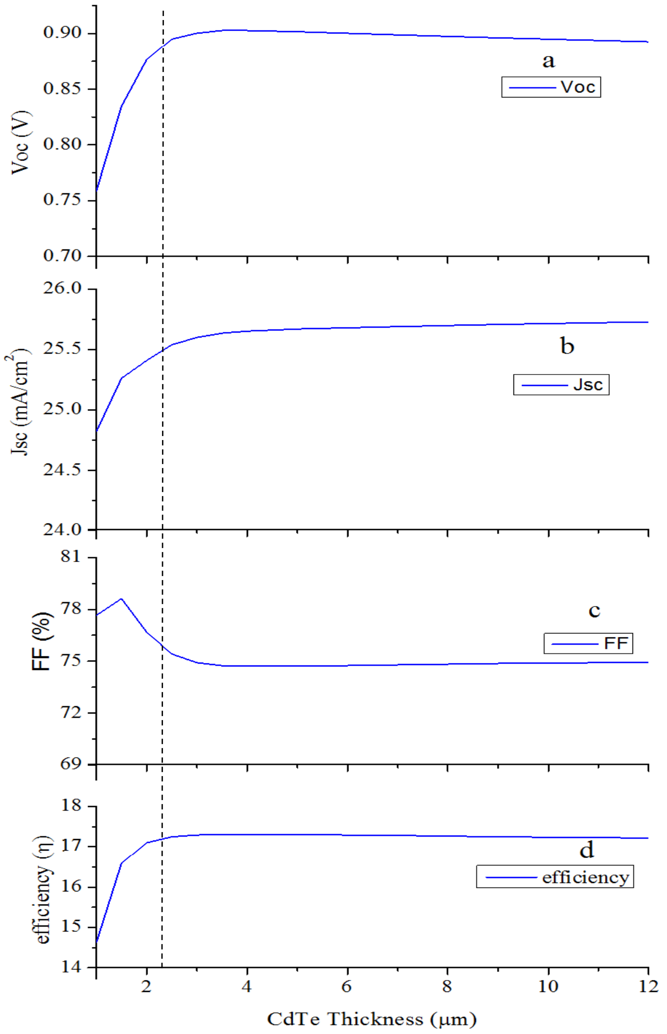

Fig.7 Effect of CdTe layer thickness variation on ITO/Cd$_{0.2}$Zn$_{0.8}$S/CdTe cell parameters without ER layer (a) *Voc*, (b) *Jsc* (c) FF and (d) efficiency

It is evident from Fig.7 that a slightly declining trend of overall efficiency was noticed after 8 μm. The reduction of efficiency might be due to the increment of the bulk series resistance of the cell beyond 8 μm thickness. Thus it was fixed at 3 μm.

C. Incorporation of ZnTe:Cu ER Layer

Finally, a 50 nm Cu doped ZnTe ER layer is inserted with the optimized ITO/Cd$_{0.2}$Zn$_{0.8}$S/CdTe/Au solar cell to explore the influence of ZnTe:Cu on cell performance. ZnTe;Cu makes a positive conduction band offset ($\Delta E_c \geq 0.72\ eV$) by which it reflects electron and reduces forward current as well as reduce interface recombination. On the other hand, a valence band offset ($\Delta E_v \geq 0.5\ eV$) occurred which impede the flow of hole. As a consequence the ZnTe:Cu layer is doped with degenerately over 1×10^{19} cm^{-3} for allowing the electron tunnelling at the back-contact interface. In Fig. 8, it is observed that with the incorporation of ZnTe:Cu layer J_{sc} increase to 27.17 mA/cm^2 and more interestingly it was noticed that the value of J_{sc} was unchanged while the absorber hole concentration increases from 2×10^{14} cm^{-3} to 3×10^{15} cm^{-3}. In the case of V_{oc}, a little decrement was found from its initial value and it continues falling upto at a hole concentration to 3×10^{14} cm^{-3} after that it increases linearly with absorber hole concentration as shown in Fig. 8 (a). After insertion of an ER layer *FF* shows incremental characteristics till 7×10^{14} cm^{-3} after that it falls sharply as illustrated in Fig. 8 (c).

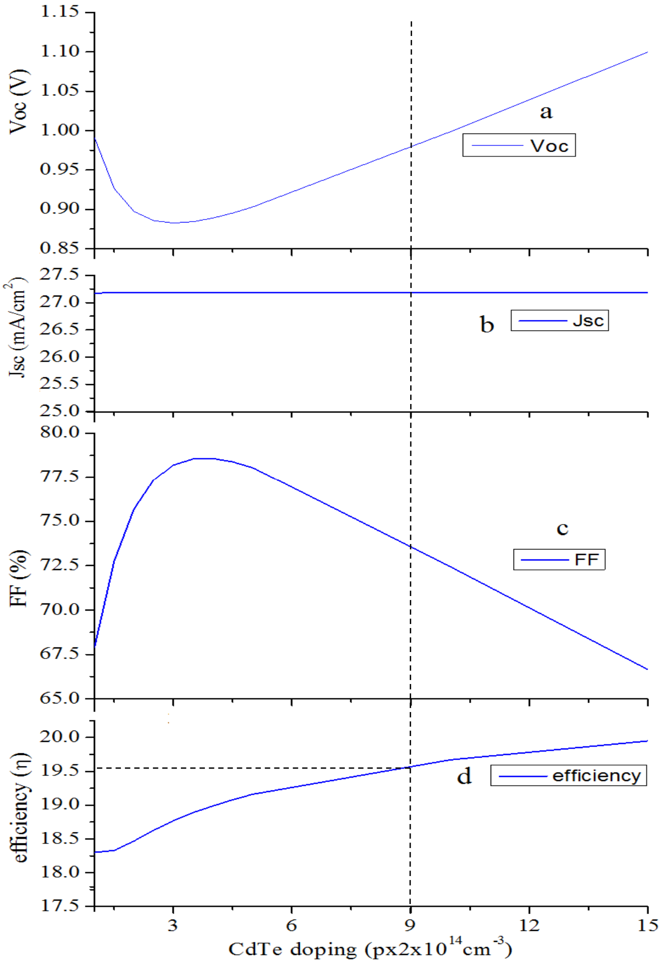

Fig. 8 Effect of CdTe layer doping concentration variation on ITO/Cd$_{0.2}$Zn$_{0.8}$S/CdTe/Au cell parameters with ZnTe:Cu ER layer (a) *Voc*, (b) *Jsc* (c) FF and (d) efficiency

Finally, the overall efficiency of the proposed cell (ITO/Cd$_{0.2}$Zn$_{0.8}$S/CdTe/ZnTe:Cu/Au) shown energy conversion efficiencies over 19 % with higher absorber hole concentration as in Fig. 8 (d). The comparative performance of the modified cell structure with base cell is presented in Table III.

TABLE III PERFORMANCE OF BASE CELL AND MODIFIED CELL

	Voc	***Jsc***	**FF**	***η***
Base Cell	0.87	24.6	76	16.4
Modified cell without ER	1.05	25.15	66.41	17.58
Modified cell with ER	1.1	27.18	66.65	19.93

It is clear from Table III that incorporation of Cd$_{1-x}$Zn$_x$S window layer in base cell increased *Jsc* and V_{oc}. Moreover, application of ZnTe: Cu ER in modified cell further improved all the cell output parameters and overall conversion efficiency.

IV CONCLUSIONS

Incorporation of Cd$_{1-x}$Zn$_x$S window in the baseline of CdS/CdTe solar cell improves the performance by enhancing

J_{sc} = 6.34% than CdS. In addition, J_{sc} in $Cd_{1-x}Zn_xS$/CdTe is less sensitive to thickness variation which allows flexibility in fabrication. Meanwhile, the V_{oc} is proportionately increased with CdTe doping densities. However, this beneficial effect was neutralized by the prominent decrement of FF as well as J_{sc}. Furthermore, the addition of Cu doped ZnTe ER mitigates this effect by reducing forward current as well as increased V_{oc} over 1 V. Moreover, ZnTe:Cu maintains the value of J_{sc} and improve FF at a doping concentration of 7×10^{14} cm^{-3}. However, after this doping concentration, decrease in FF observed. This decreased FF hinders the further improvement of cell performance with ZnTe:Cu ER. As a consequence, it can be concluded that the further improvement of the proposed cell (ITO/$Cd_{0.2}Zn_{0.8}S$/CdTe/Au) performance is strongly depends on FF enhancement in other way. It was planed that the proposed cell will be fabricated for further investigations. The final decision can be made after the proposed cell fabrication and measurements.

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