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NUMERICAL MODELING OF $Zn_xCd_{1-x}S/Zn_xCd_{1-x}Te$ SOLAR CELLS BY AMPS-1D

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ABSTRACT

Cadmium Telluride (CdTe) thin film solar cell has long been recognized as a leading photovoltaic candidate for its high efficiency and low cost. The efficiency of CdTe based solar cell can be increased using ternary material as window and absorber layer. In this study a new solar cell structure was proposed, where Zinc Cadmium Sulfide ($Zn_xCd_{1-x}S$) was used as window layer and Zinc Cadmium Telluride ($Z_xCd_{1-x}Te$) was used as an absorber layer with an added advantage of variable band gap. By varying the composition of the zinc content, the band gap was varied between 2.42-3.7eV for ZnCdS and 1.45-2.25eV for ZnCdTe respectively, thereby increasing the cell's performance in the lower wavelength region, resulting in higher efficiency. In this work the band gap of $Zn_xCd_{x-1}Te$ layer is used 1.53eV which is in the optimum range, can be achieved with Zn composition of 0.09. Incorporation of Zn can be reduced the window and absorber layer thickness significantly, which eventually will reduce the material cost, save processing time and energy required for fabrication. The numerical simulation has been performed using AMPS-1D simulator to explore the possibility of higher efficiency and stable ultra thin ZnCdS/ZnCdTe cell with suitable Back Surface Field (BSF). The performance parameters were found better in the modified cell structure. The effect of BSF layer and the operating temperature on the cell performance parameters was also investigated in this work. The cell structure of Glass/ZnO/Zn_2SnO_4/ZnCdS/ZnCdTe/ZnTe/Ni showed highest conversion efficiency of 21.17% than other cells with different BSF. The cell with Cu_2Te BSF showed better stability with TC of - 0.15%/°C in the operating temperature range from 25˚C to 40˚C. After 40˚C temperature the cell with Cu_2Te/Mo gives better stability as its efficiency remains almost unchanged in the operating temperature up to 100˚C with a TC 0.01%/˚C.

Keywords: AMPS-1D, ZnCdTe Solar Cell, BSF, Thin Film Solar Cell

1. INTRODUCTION

The CdTe thin film solar cells have shown promising efficiency (Wu et al. 2001), (Khosroabadi et al. 2014) and long-term stable performance (Batzner et al. 2001), (Yang et al. 2014) under AM1.5 illumination for global usage. However, conversion efficiencies of CdTe solar cells with homojunction have not shown encouraging results. Thus, in CdS/CdTe solar cells incorporation of zinc (Zn) in both the window layer (CdS) and absorber layer (CdTe) and insertion of a this buffer layer of Zn_2SnO_4 between TCO and window layer are very promising in order to achieve high efficiency, reliable and stable solar cells than the other counterparts (Hossain et al. 2001), (Aliyu et al. 2014). Undoubtedly one of the main goals of today's solar cell research is using less semiconductor material by making the cells thinner. Thinning will not only save material, but will also reduce production time, and the energy requires producing them. All of these aspects will decrease the manufacturing cost of cells. The CdS window layer has a lower band gap, which causes significant absorption in the short-wavelength region which is below 500 nm. Substituting $Zn_xCd_{1-x}S$ as an alternative window layer with a higher band-gap than CdS is a promising approach. In this study, $Zn_xCd_{1-x}S$ has been substituted for CdS as it can provide a more transparent window in the blue region (<500nm). As demonstrated by Oladeji et al., 2000 and several other researchers (Hussain et al. 2001), (Oladeji and Chow, 2005), the spectral response in the blue region can be significantly enhanced using $Zn_xCd_{1-x}S$ as a window layer in CdTe solar cells. Oladeji et al., 2000 showed improved Quantum Efficiency (QE) in comparison to CdS device. CdTe semiconducting material has shown great potentials as an absorber material for thin film solar cells with solar cells based on this material attaining a maximum efficiency of 16.5%. However, for this thin film technology to compete with other conventional energy sources, its efficiency needs to be improved. In an attempt towards a higher efficiency thin film solar cell structure, this study proposes the use of a ternary semiconductor cadmium zinc telluride (CdZnTe) as an absorber layer to form ZnCdS/ZnCdTe solar cell.

To improve the cell stability at higher operating temperature and further improvement of cell performance a highly doped semiconductor is deposited between ZnCdTe surface and the metal

back contact surface as a back surface field (BSF) layer. BSF layer overcome the rollover effect and reduce the loss due to the minority carrier recombination at the back contact of the ultra thin ZnCdTe cell. Thus, both open circuit voltage and short circuit current was increased by reducing the back surface recombination. As a result this proposed cell structure has shown the prospect to form a highly efficient solar cell. In this study, Zinc Telluride (ZnTe), Cupric Telluride (Cu_2Te), Arsenic Telluride (As_2Te3) and Lead Telluride (PbTe) are used as BSF materials.

2. MODELING AND SIMULATION

The purpose of numerical modeling and simulation in photovoltaic solar cell analysis is to check the validity of proposed physical structures maintaining cell geometry and cell performance. The Analysis of Microelectronic and Photonic Systems-1D (AMPS-1D) program has been used to visualize the details of the physical operation of solar cells. This simulation software has also been tested for thin film CIGS and CdTe solar cells as discussed by Degrave et al., 2003. It is perfectly simulate the electrical characteristics of the heterojunction solar cells. AMPS-1D has been also used to investigate the effect of different BSF on ultra thin film CdTe solar cells.

In this work the thin film CdS/CdTe solar cell with conventional structure (Glass/ZnO/CdS/CdTe/Cu) were chosen for modifying its structure to achieve an ultra thin high efficient solar cell. This reference structure has shown in the Fig. 1(a).

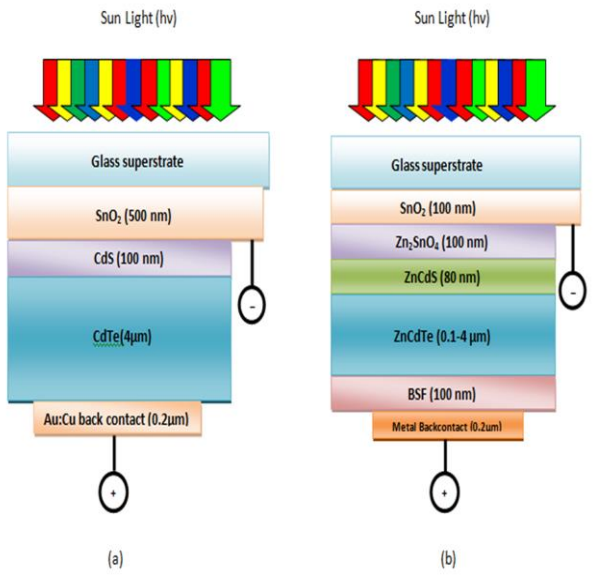

Figure 1 Structure of ZnCdTe solar cell: (a) Conventional baseline case structure and (b) modified structure for higher performance.

At the beginning, this reference cell structure has been modified by changing different layer, varying layer thickness and selecting suitable front and back contact for getting higher performance. Commercially available ITO coated glass was selected as superstrate and low resistive conducting ITO as the front contact for modified solar cell. By adding an extra Zn_2SnO_4 buffer layer in the conventional cell structure and incorporating Zn with the both CdS window layer and CdTe absorber layer, a new solar cell structure has been proposed. But the formation of stable and non-rectifying back contact to ZnCdTe is one of the major and critical problems for ZnCdTe based solar cells. Typically, metals with a high work function ($\varphi m \geq 5.9$ eV) are required to make an ohmic contact to p-ZnCdTe but most metals do not possess such high work functions. Potential metals are tried as the final metal back contact of the proposed cells, but only a few of them which are rare-earth and expensive like Te, Au, Pd and Pt show acceptable performance but others are have shown inferior cell performance. To overcome this obstacle a usual approach is to either reduce the barrier height or moderate its width by inserting a highly doping extra layer to produce back surface field (BSF) with appropriate material in between the ZnCdTe and final metal back contact. This BSF has been found to reduce the back surface recombination velocity (BSRV) and can solve back contact problem of proposed ZnCdS/ZnCdTe solar cells. And the final proposed cell structure (Glass/SnO_2 (ITO) /Zn_2SnO_4(ZTO) / ZnCdS / ZnCdTe / BSF/Back Contact) has been shown in the Fig. 1 (b).

Four layers that were highlighted in this analysis are the n-Zn_2SnO_4 buffer layer, n-$Zn_xCd_{1-x}S$ window layer, p-ZnCdTe absorber layer and p-doped BSF layer. The ZnCdTe absorber layer thickness was varied from 0.1 μm to 4 μm and the other layers thickness were fixed to the optimum values found in literature (Nowshad et al. 2010). It was a tough challenge to select the appropriate parameters to be used for the individual layers of the cells. Many of them depend on fabrication processes and deposition techniques and can thus vary even between devices fabricated at the same chamber. The dependability of this analysis, of course relies on the selection of the material parameters that are going to be used in the simulation. Table 1 shows the material parameters used in this modeling, which were chosen based on experimental data, literature values, and theoretical study.

3. RESULTS AND DISSCUSSION

3.1. Optimizition of $Zn_xCd_{1-x}S$ window layer:

A simple structure of baseline case of CdTe cell was chosen as the starting point of the analysis in which CdS was replaced by $Zn_xCd_{1-x}S$ and CdTe was replaced by $Zn_xCd_{1-x}Te$. In this analysis the band gap of $Zn_xCd_{1-x}Te$ layer is used 1.53eV which is in the optimum range, can be achieved with Zn composition at x=0.09. The optimum range of 'x' value in absorber layer of

$Zn_xCd_{1-x}Te$ has been taken from reference (Imamzai et al. 2014a), (Imamzai et al. 2014b), (Schlesinger et al. 2001), and detailed study of window layer of $Zn_xCd_{1-x}S$ has been analysed in this work.

Numerical simulation has been done to see the effect of Zn content of $Zn_xCd_{1-x}S$ window layer on conversion efficiency from x=0 to x=1 using the parameters related to electrical and optical behavior of $Zn_xCd_{1-x}S$ which was adopted from literature reviews and after simulation.

Table 1 Material parameters used in AMPS simulation

Param.	SnO_2	Zn_2SnO_4	ZnCdS	ZnCdTe	As_2Te_3/PbTe/ZnTe/Cu_2Te
W [nm]	100	100	80	1000	100
$\varepsilon/\varepsilon_0$	9	9	10	10.2	20/20/14/10
μ_n [cm^2/Vs]	100	32	100	250	500/6000/70/500
μ_p [cm^2/Vs]	25	3	25	70	210/4000/50/100
n, p [cm^{-3}]	n: $l0^{17}$	n: 10^{19}	n: 2.5×10^{16}	p: 5.0×10^{14}	P:$6.8x10^{19}$/$5x10^{21}$/$7.5x10^{19}$/10^{20}
E_g [eV]	3.6	3.35	2.5	1.53	0.6/0.32/2.25/1.18
N_c [cm^{-3}1	2.2×10^{18}	2.2×10^{18}	2.2×10^{I8}	1.5×10^{17}	$5x10^{18}$/$7.5x10^{17}$/$7.8x10^{17}$/$7.5x10^{17}$
N_v [cm^{-3}]	$l.8\times10^{19}$	1.8×10^{19}	1.8×10^{19}	1.8×10^{18}	$1.8x10^{19}$/$1.5x10^{19}$/$1.6x10^{19}$/$1.5x10^{19}$
X (eV)	4.5	4.5	4.46	4.4	4.0/4.6/3.65/4.2

For the value x>0.08 the resistivity of $Zn_xCd_{1-x}S$ layer is very high which eventually decreases all the performance parameters i.e. Jsc, Voc, Eff and FF which is shown in the Fig. 2. The value of Voc is suddenly dropped in the range of Zn content from x=0.08 to x= 0.1 and gradually decreasing onward due to high resistivity of $Zn_xCd_{1-x}S$ with increasing x value up to x=0.6. After x=0.6 the ZnCdS/ZnCdTe interface the electron affinity, lattice constant and thermal matching result in the formation of high quality of interface states which increases the Voc of the cell (Chu, 1985), however, other parameter Jsc, FF, Eff% gradually in decreasing trend due to resistivity increasing from 1 Ω-cm to 10^{10} Ω-cm with increasing zinc content in the compound cannot be overlooked (Burton and Hench, 1976). So, x=0.08 was selected as it showed reasonable cell output parameters (Jsc, Voc, Eff and FF) with high conversion efficiency of the cell as well as lower resistivity of the $Zn_xCd_{1-x}S$ layer. In this part of work, the 80 nm $Zn_{0.08}Cd_{0.92}S$ layer will be optimized for higher cell performance. Fig. 3 shows the effects in details of $Zn_{0.08}Cd_{0.92}S$ (optimum value of x=0.08) window layer thickness variation from 25 nm to 200 nm on the cell output parameters such as Jsc, Voc, and FF and conversion efficiency from AMPS calculation. With low thickness of window layer (< 80 nm), the cell performance degraded due to pinhole formation in the window layer and for high thickness of window layer (>80 nm), the interface state of window (ZnCdS) and absorber layers is quite good which result the better performance of the cell.

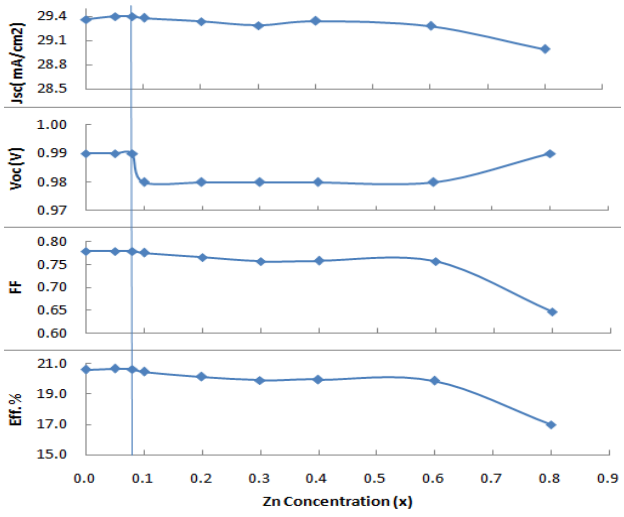

Figure 2 Effect of Zn content (x) in $Zn_xCd_{1-x}S$ thin film on the proposed cell performance

The conversion efficiency of the baseline case cell was found 17.88% (Voc=0.90V, Jsc=26.58mA/cm^2, FF=0.81), where 4µm CdTe absorber layer, 100nm of CdS window layer, 500nm of SnO_2 front contact and Cu as final back contact metal were used. When introducing 100nm Zn_2SnO_4 buffer layer between the 100nm SnO_2 front contact and 80nm of $Zn_xCd_{1-x}S$ window layer along with 1µm $Zn_xCd_{1-x}Te$ absorber

layer the conversion efficiency increased to 18.09% (Voc=0.93V, Jsc=30.15mA/cm^2, FF=0.70). The improvement of efficiency is resulted from higher Jsc as the $Zn_xCd_{1-x}S$ window layer improves the absorption of photon energy in the short wavelength region (blue region).

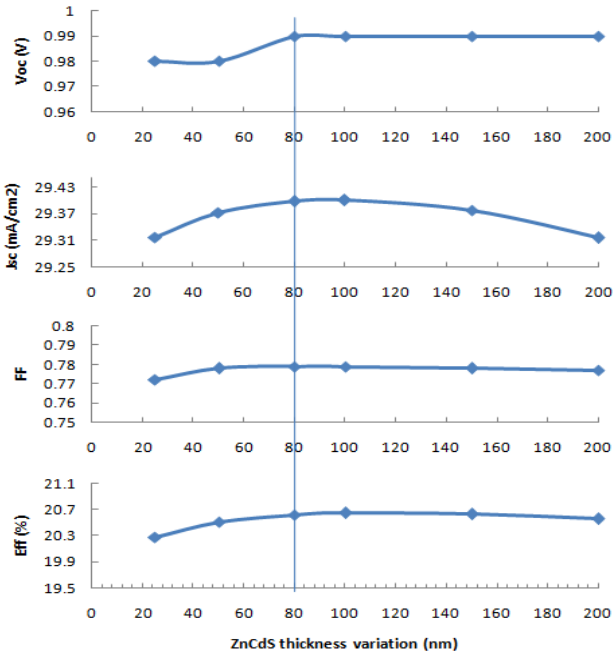

Figure 3 Effect of $Zn_{0.08}Cd_{0.92}S$ (optimum x=0.08) thickness on ZnCdS/ZnCdTe cell parameters

The spectral response (SR) of $Zn_{0.08}Cd_{0.92}S$ window layer for thickness variation from 25 nm to 200 nm is shown in Fig. 4. It can be seen from Fig. 4 that, when the wavelength is below 510 nm the quantum efficiency (QE) is slight affected with the increasing $Zn_{0.08}Cd_{0.92}S$ layer thickness which influences the cell Jsc and finally conversion efficiency. The high SR for low thickness of window layer was for high transparency of the ZnCdS layer.

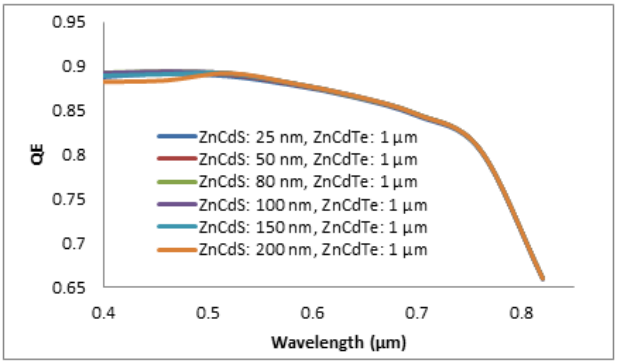

Figure 4 Effect of $Zn_{0.08}Cd_{0.92}S$ thickness on proposed cell quantum efficiency (QE)

3.2 Analysis of BSF layer and cell stability:

One of the major differences of thin cells compared to the thicker ones is that the absorber/back contact interface is located closer to the p-ZnCdTe and n ZnCdS junction and the choice of the back contact material therefore has a high impact on the cell performance. A stable back contact that is not significantly rectifying is essential for good performance and long term stability of ZnCdS/ZnCdTe cells. The formation of a low resistance, low barrier back contact is one of the most challenging aspects for high performance ZnCdTe solar cells. In general, the structure with BSF layer (Fig. 1(b)) showed higher Voc, FF, Jsc and η than the cell without BSF. In this work all the cell with BSF layer showed higher efficiency (η), Voc and FF but poor Jsc due to supper thinning (≤.6µm) of ZnCdTe material and low resistance as well as low barrier back contact formation which showed the Fig. 5.

In this analysis the cell structure with ZnTe/Ni layer has shown higher performance than As_2Te_3, PbTe and Cu_2Te BSF with 1µm ZnCdTe layer which is listed in Table 2. But in particular with ZnTe BSF the cell with 0.6 µm ZnCdTe layer showed highest conversion efficiency of 21.17% and moderate FF of 0.781. However, the cell structure without BSF showed highest FF of 0.817 and lowest conversion efficiency of 17.88 due to low value of Voc of 0.90% for high resistance as well as high barrier back contact in the absorber/back contact interface of the cell.

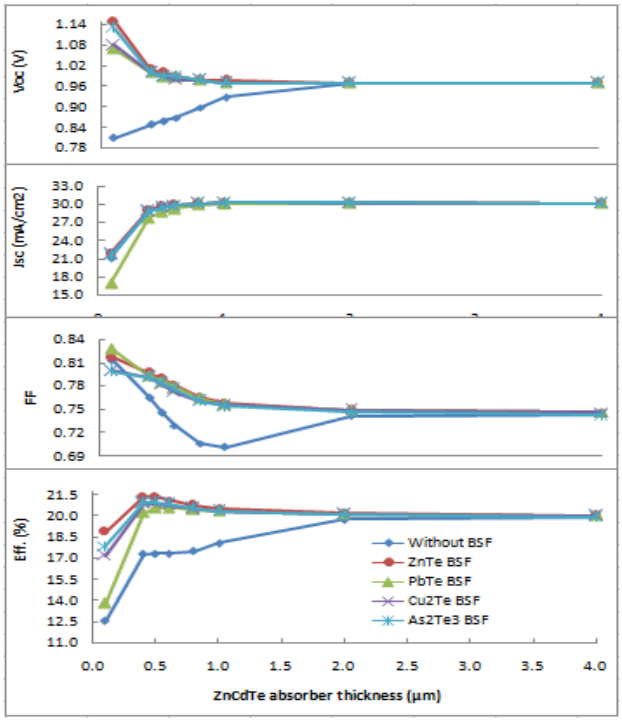

Figure 5 Effect of ZnCdTe layer thickness on cell performance parameters of proposed cells with and without BSF.

Table 2 Output parameters of the proposed cell structures

Cell structure	Eff (%)	FF	Jsc (mA/cm_2)	Voc (V)
Glass/ZnO/CdS/CdTe/Cu	17.88	.81	26.579	.90
Zn_2SnO_4/ZnCdS/ZnCdTe/Te	18.09	.70	30.159	.93
PbTe BSF	20.63	.78	29.945	.98
As_2Te_3 BSF	21.02	.78	29.893	.99
Cu_2Te BSF	20.88	.78	29.945	.98
ZnTe BSF	21.17	.78	30.037	.99

The J-V characteristics of the cells with BSF and without BSF, all with 0.6 µm ZnCdTe, 80 nm ZnCdS and same front contact are shown in Fig. 6 to compare each structure of the proposed cell performance. The Voc and Jsc increase for cell with BSF than without BSF due to ohmic contact formation in the absorber/back contact interface of the cell with BSF than schottky contact of the cell without BSF.

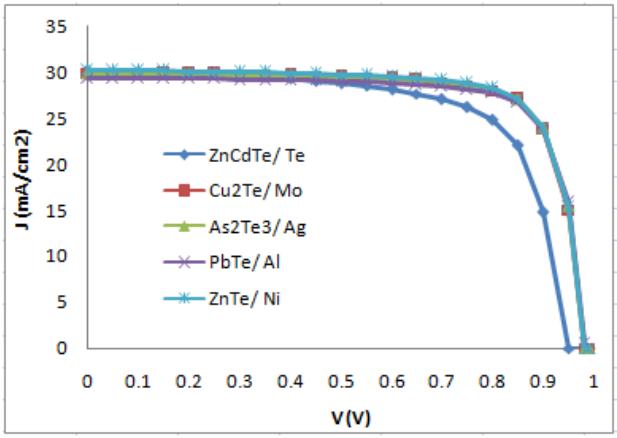

Figure 6 J-V characteristics of the proposed cells structure.

Before drawing the final conclusion on BSF choice there is a need to compare the stability of the cells at higher operating temperature with BSF. As it is well known that operating temperature plays a very important role on the cell output performance in practical fields where the operating temperature is higher than 25°C. At higher operating temperature, cell properties are affected as also found in this analysis. A comparison was done at operating temperature ranged from 25°C to 100°C for all the cells with 0.6 µm ZnCdTe, 80 nm ZnCdS layer and with same front contact (ITO/ZTO). The results obtained from AMPS calculation are shown in Fig. 7.

From the Fig. 7 it is clear that cell conversion efficiency without BSF layer linearly decreased with the increase of operating temperature with a temperature coefficient (TC) of -0.26%/°C, which is in good agreement with related works (Matin et al. 2013). The cell with ZnTe BSF showed better stability with TC of - 0.18%/°C in the operating temperature range from 25˚C to 40˚C. After 40˚C temperature the cell with ZnTe/Ni gives better stability as its efficiency remains almost unchanged in the operating temperature up to 100˚C with a TC 0.04%/˚C. Cells with Cu_2Te/Mo gives better stability as its efficiency remains almost unchanged in the operating temperature range from 40°C to 100°C. But in the operating temperature range from 25°C to 40°C its efficiency decreases with a TC of -0.15%/°C. The stability of cell with As_2Te_3/Al is almost similar to that without BSF and which is -0.25/˚C. Another cell with PbTe/Ag shows similar temperature coefficient of cell with As_2Te_3/Al. However, the performances of the cells with Cu_2Te BSF have shown better stability than all other cells. There are good indications of Cu_2Te and ZnTe BSF layer for higher efficiency and ultra thin cell stability in comparison to other related published work (Aliyu et al. 2010), (Nowshad et al. 2010), (Matin et al. 2013). The stability of cells with BSF increases than the cell without BSF might be due to good interface state at the absorber/back contact interface for converting schottky contact to ohmic contact.

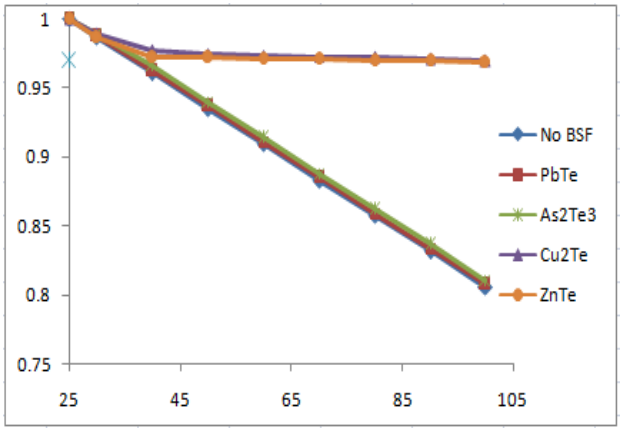

Figure 7 Effect of operating temperature on the proposed cells

Comparison between recent published work and the proposed work:

From the comparison table below, it is seen that the proposed work is much better than the recent published works in comparison open circuit voltage (Voc), shot circuit current (Jsc), conversion efficiency (Eff%) and stability (TC%) of the cell structure. The superior performance of Glass/ITO/Zn2SnO4/ZnCdS/ZnCdTe/ BSF/Backcontact cell structure is due to high Jsc and Voc which collectively contributes to the higher conversion efficiency. The low value of FF might be due defect states in any of the layer in the full device. Nevertheless, the 21.17% efficiency of $Zn_{0.08}Cd_{0.92}S$/ ZnCdTe solar cells outcomes in this work is much higher than 20.78% of CdS/CdTe cell structure (Matin et al. 2013), 18.6% of CdS/CdTe cell structure (Nowshad et al. 2010) and 20.4% of CdS/CdZnTe cell structure (Aliyu et al. 2010).

In comparison to stability with respect to temperature coefficient (TC%) the proposed solar cell structure with As_2Te_3, ZnTe, PbTe and Cu_2Te BSF show better stability than the solar cell structure in recent published work shown in the table above. Our design approach then represents the right approach if the proposed cell structure can be fabricated a commercialized successfully.

Table 3 Comparison between recent published work and the proposed work

This work and published work	BSF Material	Voc (V)	Jsc (mA/cm²)	FF	E_{ff} (%)	TC (%/°C)
Matin et al., 2013	ZnTe	0.960	25.63	74.4	18.37	-0.3
Matin et al., 2013	As2Te3	0.990	24.73	84.5	20.78	-0.4
Matin et al., 2013	Cu2Te	0.990	24.73	79.8	19.54	-0.35
Nowshad et al. 2010	ZnTe	0.90	24.92	0.70	15.8	-0.3
Nowshad et al. 2010	As2Te3	0.92	24.97	0.81	18.6	-0.4
Aliyu et al., 2010	-	0.96	24.90	0.86	20.4	-
Proposed work	As_2Te_3	0.99	29.893	0.776	21.019	-0.25
Proposed work	Cu_2Te	0.98	29.945	0.773	20.877	-0.15, (25°-40°C) -0. 01, (40°-100°C)
Proposed work	ZnTe	0.99	30.037	0.781	21.172	-0.18, (25°-40°C) -0. 005, (40°-100°C)
Proposed work	PbTe	0.98	29.945	0.773	20.626	-0.26

4. CONCLUSION

The main aim of this analysis was to introduce a new cell structure where ZnCdS and ZnCdTe are used as window absorber layer respectively. This modified cell structure shows higher performance than baseline cell structure. The conversion efficiency of conventional cell was found 17.88% whereas proposed cell shows conversion efficiency 18.19%. Another target of this analysis was thinning of ZnCdTe absorber layer to the stream limit without affecting the overall cell performance. But the conversion efficiency shows a slight decreasing trend with a decrease of the ZnCdTe thickness up to 0.5µm. The overall performance of the ZnCdS/ZnCdTe cell was affected by the back surface recombination in case of thinner ZnCdTe absorber.

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