Ultra Thin High Efficiency CdS/CdTe Thin Film Solar Cells from Numerical Analysis

M. A. MATIN¹, NOWSHAD AMIN^{1,2} AZAMI ZAHARIM^{2,3} AND KAMARUZZAMAN SOPIAN² ¹Department of Electrical, Electronics and System Engineering, ²Solar Energy Research Institute ³Head Centre for Engineering Education Research Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia, 43600 Bangi, Selangor, MALAYSIA mamatin@eng.ukm.my, nowshad@eng.ukm.my, azaminelli@gmail.com,ksopian@eng.ukm.my

Abstract: - Polycrystalline cadmium telluride (CdTe) is the leading material for realization of low cost and high efficiency solar cell for terrestrial use. In this work, the CdTe conventional structure [1] was investigated and achieved the maximum conversion efficiency of 13.2% with CdTe baseline structure of SnO₂/CdS/CdTe. To explore the possibility of ultra thin and high efficiency CdS/CdTe solar cell, the CdTe absorber layer and CdS window layer were decreased and found that 1 µm thin CdTe layer showed reasonable range of efficiency. Moreover, it was found that there were scopes to increase cell efficiency by reducing the cadmium sulfide (CdS) window layer thickness. The CdS window layer was reduced to 60 nm with insertion of zinc oxide (ZnO) or zinc stannate (Zn₂SnO₄) as a buffer layer to prevent forward leakage current. All the simulation have been done using Analysis of Microelectronic and Photonic Structures (AMPS 1D) simulator. The maximum conversion efficiency of 18.3% (*Voc* = 1.00 V, *Jsc* = 26.15 mA/cm², FF = 0.769) was achieved with 1 µm-CdTe absorber layer, 60 nm-CdS window layer and 100 nm of ZnO or Zn₂SnO₄ buffer layer. Moreover, it was found that the cell normalized efficiency linearly decreased with the increasing operating temperature at the gradient of -0.4%/°C, which indicated better stability of the CdS/CdTe solar cells.

Key-Words: - Thin film solar cell, high efficiency, CdTe, CdS, zinc oxide, zinc stannate, AMPS 1D

1 Introduction

Thin-film polycrystaline CdTe based solar cells are one of the most promising candidates for photovoltaic energy conversion because of the great potential of low cost, high efficiency, reliable and stable thin film solar cell fabrication. First, the cell is produced from polycrystalline materials and glass, which are potentially much cheaper than other counter parts. Second, the polycrystalline layers of a CdTe solar cell can be deposited using a variety of different low cost techniques, such as close-space sublimation (CSS), chemical vapor deposition (CVD), chemical bath deposition (CBD), and spluttering. Third, CdTe has a high absorption coefficient over 5×10^{5} /cm, which means that all the potential photons with energy greater than the bandgap can be absorbed within few µm of CdTe absorber layer. And finally, CdTe has a direct optical bandgap of 1.45 eV which is very close to the optimum bandgap for solar cells. Hence, the small thickness required for an absorbing layer makes the cost of material for CdTe solar cells relatively very low. Clearly 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 lower production time, and the energy need to produce the solar cell. All of these factors will decrease the production cost. Moreover, the CdTe thin film solar cells have shown long-term stable performance and high efficiency under AM1.5 illumination for terrestrial uses.

of However. conversion efficiencies homojunction CdTe solar cells have not been encouraging results. Thus, heterojunction cell structure with wide band-gap n-type semiconductor (commonly CdS) and p-CdTe are widely used. From optoelectronic and chemical properties, CdS is the best suited n-type hetero-junction partner to CdTe for high-efficiency and low-cost cells. The maximum theoretical efficiency for its band gap (1.45 eV) and a standard solar spectrum is about 29%. In 1982, Tyan et al. published an interesting paper on CdTe/CdS thin film solar cells reporting an efficiency of 10% [2]. Afterwards an efficiency of 15.8% has been reached by Ferekides et al. [3]. Finally a group of NREL researchers reported a record efficiency of 16.5% [4]. This 16.5% efficient CdS/CdTe cell used modified cell structure of CTO/ZTO/CdS/CdTe with 0.1 µm CdS and 10 µm of CdTe layer fabricated using three different technology CSS for CdTe film, CBD for CdS film and magnetron sputtering for all other layers. This champion cell efficiency (16.5%) is a little over half of the 29% theoretical limit, but it was estimated that practical CdTe devices with 18-19% efficiencies should be feasible in the near future [5]. However, there are scopes to improve the CdS/CdTe solar cell performance further more by modified design and simple deposition technique to improve any one of cell output parameters. It has been observed that CdS/CdTe cells are suffering from low open circuit voltage (V_{oc}) then its counterparts. The largest contribution to the efficiency difference with the same bandgap material like GaAs is the V_{ac} , where the value of the record CdTe cell is about 230 mV below the GaAs cell. The analogous voltage difference for the other major thin-film polycrystalline solar cell, Cu(In,Ga)Se₂ (CIGS), is only about 30 mV when compared to crystalline silicon. If the CdTe voltage deficit were reduced to the same 30 mV, with the same current and fillfactor, CdTe cells would achieve the efficiency about 22%. The reason for the relatively low voltage of CdTe solar cells is a combination of low carrier density (~10¹⁴ cm⁻³) and low absorber lifetime (generally below 1 ns). In practice, the voltage may be further compromised by higher carrier density $(\sim 10^{16} \text{ cm}^{-3})$ and higher absorber lifetime (more than 1 ns) and by reducing the significant back-contact barrier height. The strategies for improving voltage and cell performance have been explored utilizing AMPS 1D (Analysis of Microelectronic and Photonic Structures) simulator and have also been discussed in this work.

2 Modeling and Simulation

Fig. 1 illustrates the CdTe baseline case structure and the modified (Glass/SnO₂/ZnO(Zn₂SnO₄)/CdS/CdTe/Ag) structure of CdTe cell for higher conversion efficiency (η). It is clear from Fig. 1 that the new structure has an extra layer (ZnO or Zn₂SnO₄) in between TCO and CdS layer to achieve ultra-thin CdS window layer for better performances and thinner CdTe layer. Thus, the front contact consists of TCO plus a buffer layer. The doping concentration (~10¹⁴ cm⁻³) used in the baseline case has been changed to (~10¹⁶ cm⁻³) more effective and today's practically achievable values for higher efficiency. Considering the low cost feature Ag is used as back contact material with back contact barrier height (Φ_{bL}) of 1.25 eV instead of Au (Φ_{bL} = 0.4 eV) in the modified structured cell.



Fig. 1: Structures of the CdTe solar cells: (a) Conventional baseline case structure and (b) Modified structure for higher conversion efficiency.

In this work, AMPS 1D was used to explore the conventional CdTe baseline cell and modified structured cells for achieving thinner CdTe and CdS layers with higher conversion efficiency. This AMPS program has been developed to realistically simulate the electrical characteristics of the thin-film heterojunction solar cells. It has been tested for thinfilm CdTe and CIGS solar cells [6]. Four basic layers that have been emphasized in this modeling are the buffer layer (Zn₂SnO₄), n-CdS layer, p- $CdS_{x}Te_{1-x}$ layer (developed in film growth process of CdTe as in CSS), and p-CdTe layer. Table 1 shows all the material parameters used in this modeling, which were selected based on literature values, theory, or in some case, reasonable estimations.

In this analysis, we have varied the CdTe layer thickness from 10 nm up to 10 μ m, CdS window layer thickness from 10 nm to 500 nm and ZnO and Zn₂SnO₄ buffer layer thickness from 10 nm to 500 nm by keeping all other parameters at fixed value as shown in Table 1 aiming to efficient and thinner CdS/CdTe solar cell.

	n-ZnO/ Zn ₂ SnO ₄	n-CdS	p-CdS _x Te _{1-x}	p-CdTe
W (µm)	0.01-0.5	0.02-0.5	0.0-0.5	0.1-10
ε/εο	9.0	9.0	9.4	9.4
$\mu_{\rm c} ({\rm cm}^2/{\rm Vs})$	32	350	500	500
$\mu_p (cm^2/Vs)$	3	50	60	60
n, p (cm ⁻³)	10 ¹⁹	10 ¹⁸	10^{14}	10 ¹⁶
E _g (eV)	3.35	2.42	1.41	1.45
$N_{\rm C}$ (cm ⁻³)	2.2×10^{18}	2.2×10^{18}	7.5×10^{17}	7.5×10^{17}
$N_V (cm^{-3})$	1.8×10^{19}	1.8x10 ¹⁹	1.8×10^{19}	1.8x10 ¹⁹
χ (eV)	4.50	4.50	4.28	4.28

Table 1 Material parameters used for cell simulation.

3 Results and Discussion

In this work, first of all the conventional CdTe baseline structure (SnO₂/CdS/CdTe) has been investigated and found the maximum conversion efficiency of 13.2% (*Voc* = 0.85 V, *Jsc* = 26.8 mA/cm², FF = 0.63) with 4 μ m CdTe absorber layer, 100 nm-CdS window layer and with Φ_{bL} =1.25 eV. It has been found that the conversion efficiency increases up to 15.4% (*Voc* = 0.92 V, *Jsc* = 25.76 mA/cm^2 , FF = 0.71) with the new CdTe doping concentration (5×10^{16}) and adopted life time (1.6 ns)parameters mainly due to the improvement of Voc and FF. Theoretically the minimum thickness required for CdTe films to absorb 99% of the incident photons with energy greater than Eg is approximately 2 µm [4]. But to date almost all the high efficient CdTe solar cells have been fabricated with more than 5 µm thick CdTe layer. However, further numerical analysis has been done aiming to conserve the material required and cost in CdS/CdTe solar cells by reducing the thickness of CdTe and CdS layers. The CdTe thickness has been varied from 0.01 µm to 10 µm to explore thinner absorber layer and the results obtained from AMPS simulation are shown in Fig. 2.



It is clear from the Fig. 2 that all the solar cell output parameters are almost constant above the CdTe thickness of 2 µm. The short circuit current density (Jsc) slowly decreased but the Voc and FF remains unaffected with the reduction of CdTe thickness until 1 µm but bellow 1 µm of CdTe thickness all the cell output parameters decreased. As a result the η shown very slow decreasing nature with the reduction of CdTe thickness until 1 µm and bellow 1 µm of CdTe thickness decreases rapidly which indicates that 1 µm thick CdTe cell is possibilities with very small decrease or loss in efficiency. The 1 μ m thick CdTe cell shows η of 14.6% (Voc = 0.92 V, $Jsc = 24.6 \text{ mA/cm}^2$, FF = 0.706), which indicates that with only 25% CdTe absorber material of the baseline cell loss of η is only 0.8% (15.4% to 14.6%). These results are in good agreements with related published results by SCAPS software for CdTe cells [7].

The spectral response of the above CdTe baseline case cell $(SnO_2/CdS/CdTe)$ with different CdTe layer thickness from quantum efficiency (QE) calculation by AMPS 1D is shown in Fig. 3. It is evident from Fig. 3 that the spectral response start decreasing in the operating wavelength of 460 nm to 820 nm with decreases of the CdTe layer thickness. However there are possibility of increasing QE and as well as the cell efficiency if the CdS window layer thickness (100 nm) can be reduced further

more with proper buffer layer in between TCO and CdS layer.



Fig. 3: Effect of CdTe thicknesses on the cell QE.

Before inserting buffer layer it was observed that the cell output parameters are strongly dependent on p- CdS_xTe_{1-x} layer thickness (which is unintentionally and automatically developed in the CSS film growth process). The CdS_xTe_{1-x} layer thickness depends on CSS growth time which can be reduced in the real fabrication process. In order to investigate the thickness effects of CdS_xTe_{1-x} layer on the cell performances CdS_xTe_{1-x} layer has been varied from 0 nm to 500 nm. The results obtained from AMPS are shown in Fig. 4.



Fig. 4: Effect of CdS_xTe_{1-x} thicknesses on the cell characteristics.

It can be observed from Fig. 4 that the solar cell output parameters are strongly dependent on $CdS_{x}Te_{1-x}$ thicknesses below 70 nm but above 100 nm it is not much affected. In order to take the

fabrication challenges the CdS_xTe_{1-x} layer thicknesses was selected 10 nm with the conversion efficiency of 16.82% (*Voc* = 1.00 V, *Jsc* = 24.16 mA/cm², FF = 0.765). The η improvement achieved mainly due to the improvement of *Voc* and FF but again Jsc is reduced a bit.

When the CdS film thickness has been reduced to explore thinner CdS layer, the absorption loss in the blue region due to thick CdS layer also reduces, which improves mainly *Jsc* and η . Fig. 5 shows the effects in details of CdS layer reduction from 20 nm to 200 nm on the cell all output parameters such as *Jsc, Voc, FF* and η from AMPS 1D simulation, when utilizing all the baseline parameters with CdTe layer thickness of 1 µm and CdS_xTe_{1-x} layer thickness of 10 nm.



Fig. 5: Effect of CdS film thickness on cell output parameters.

Fig. 5 shows that *Jsc* improved greatly with reduced CdS layer but *Voc* not affected and *FF* affected a little bit only. Thus, from the combined effect on η , finally the η increased with reduced CdS layer. The QE of CdS layer thickness variation from 20 nm to 300 nm from AMPS simulation is shown in Fig. 6. It is clear from Fig. 6 that when the wavelength is below 510 nm the quantum efficiency is affected much more with the increasing CdS layer thickness. This affects *Jsc* and FF and finally the conversion efficiency. This result are in good agreements with other literatures [8]. However, to date, it is impractical to fabricate good quality devices with

CdS film thickness below 60 nm by CBD process that we have selected for the fabrication of this layer. For fabrication limitation we have selected the CdS film thickness of 60 nm with η of 16.9% (*Voc* = 1.00 V, *Jsc* = 24.26 mA/cm², FF = 0.764). The η improvement achieved mainly due to the improvement in *Jsc*.



Fig. 6: Effect of CdS thicknesses on the cell QE.

In order to achieve better performance of the CdTe cell the CdS layer has been reduced to 60 nm but this reduced CdS layer will allow forward leakage current to front contact throw pinhole in CdS layer. In order to prevent this unwanted forward leakage current a high resistive buffer layer of suitable material must be inserted in between front contact TCO and CdS window layer. Further numerical analysis has been done aiming to improve the conversion efficiency of the conventional CdTe baseline case solar cell by inserting a suitable buffer layer. It is possible to take advantage of the different properties of two TCOs by forming a buffer layer. High-efficiency CIGS and CdTe devices are generally fabricated with such buffer layer structures. Now the front contact consisting of a highly conducting layer (SnO₂) for low-resistance due to contact and lateral current collection and a much thinner high-resistivity layer (called buffer layer) of a suitable material. By incorporating 100 nm thick or less a resistive buffer layer of In₂O₃, ZnO, or Zn₂SnO₄, the CdS layer thickness can be reduced <50 nm, which significantly improves the blue response of the CdS/CdTe devices. The presence of the smoother high-resistive buffer layer also improves the CdS film morphology by providing large grains during CBD. Among many potential buffer layer materials ZnO and Zn₂SnO₄ has been tried in this work. The ZnO/Zn₂SO₄ as a buffer layer has been inserted in the designed CdTe cell with CdTe layer thickness of 1 µm and CdS_xTe_{1-x} layer thickness of 10 nm, CdS layer thickness of 60 nm and with all other base parameter as in Table 1, the J-V characteristics

obtained by AMPS simulation are shown in Figure 7.



Fig. 7: Effect of ZnO and Zn₂SO₄ on the solar cell I-V characteristics.

The ZnO insertion shows almost the same results as with Zn₂SO₄ insertion. The simulation also shows that the solar cell output characteristics are independent with ZnO/Zn₂SO₄ thickness from 20 nm up to 500 nm. Moreover, it was also found that the spectral response has no effect for ZnO/Zn₂SO₄ thickness variation from 20 nm to 500 nm. Considering the reality in fabrication, we have selected the ZnO/Zn₂SO₄ buffer layer thickness of 100 nm with best conversion efficiency of 18.3% $(Voc = 1.00 \text{ V}, Jsc = 26.15 \text{ mA/cm}^2, \text{FF} = 0.769).$ The improvement in η 0f 1.4% has come from the improvement in Jsc about 0.9 mA/cm^2 than without the buffer layer. Fig. 8 shows the band diagram of finally selected cell configuration of the with Glass/SnO₂/Zn₂SnO₄/CdS/CdTe/Ag illumination at 0 V to investigate the band bending.



Fig. 8: The band diagram of the modified designed cell (Glass/SnO₂/Zn₂SnO₄/CdS/CdTe/Ag).

It is evident from Fig. 8 that there is rectifying contact at the back with p-CdTe and Ag material which may be responsible of rollover of the cell. One of the major differences in thin cells compared to the thicker ones is that the absorber/back contact interface is now located closer to the p-n 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 CdS/CdTe solar cells. The formation of a low resistance, low barrier back-contact is one of the most challenging aspects for high performance CdTe based solar cells.

Fig. 9 shows the Electric field of the final cell configuration of $Glass/SnO_2/Zn_2SnO_4/CdS/CdTe/Ag$ with illumination at 0 V to investigate the performance.



Fig. 9: Effect of electric field on the solar cell characteristics.

It is clear from Fig. 9 that the cell has a negative spike at the interface of $SnO_2/Zn_2SnO_4(ZnO)$ and positive spike at the interface of $ZnO(Zn_2SnO_4)/CdS$ and CdS/CdTe. The ZnO insertion produced larger spike than Zn_2SnO_4 insertion proving the presence of higher electric field.

In real cases operating temperature plays a very important role which affects the performance of the solar cells. At higher operating temperature, parameters such as the effective density of states, absorption coefficients, electron and hole mobility, carrier concentrations and band gaps of the materials are affected. An investigation has been done to understand the effect of temperature on cell conversion efficiency with operating temperature ranged from 25°C to 100°C as shown in Fig. 10.



Fig. 10: Effect of operating temperature on normalized efficiency.

It is evident from the Fig. 10 that the conversion efficiency linearly decreases with the increase of operating temperature at a temperature coefficient (TC) of $-0.4\%/^{\circ}$ C, which also indicates the degree of stability of the cell at higher operating temperature or in stressed conditions.

4 Conclusion

A highly efficient 18.3% (Voc = 1.00 V, Jsc = 26.15 mA/cm^2 and FF = 0.769) ultra thin CdS/CdTe solar cell has been obtained from numerical analysis with CdTe thickness of 1 µm and CdS thickness of 60 nm. The Voc and FF increased to 150 mV and 14%, respectively but *Jsc* reduced of 0.65 mA/cm² from the CdTe baseline case. It was found that 1 µm thick CdTe layer is possible with the least sacrifice of efficiency (0.8%) from the CdTe baseline case $(SnO_2/CdS/CdTe)$ of 4 μ m thick CdTe. Moreover a potential idea was found to increase the cell efficiency by reducing CdS window layer thickness by inserting suitable buffer layer. The efficiency improvement up to 18.3% has been achieved from 100 nm Zn₂SO₄ buffer layer insertion to reduced CdS window layer thickness to 60 nm which improves the QE of the cell at the blue region. The Zn₂SO₄ buffer layer insertion showed almost the same results with ZnO insertion. Moreover, the simulation result of cell operating temperature has shown the stability to some extent of this cell at higher operating temperatures. Efficient and costeffective ultra-thin film CdS/CdTe solar cell can be realized with 60 nm of CdS layer, 1 µm of CdTe layer and 100 nm of Zn₂SO₄ buffer layer.

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