A Study towards the Possibility of Ultra Thin CdS/CdTe High Efficiency Solar Cells from Numerical Analysis

M. A. MATIN¹, NOWSHAD AMIN^{1,2} AZAMI ZAHARIM³ AND KAMARUZZAMAN SOPIAN⁴ ¹Department of Electrical, Electronics and System Engineering, Faculty of Engineering And Built Environment, ²Solar Energy Research Institute, ³Head for Renewable Energy Resources and Social Impact Research Group Solar Energy Research Institute, and Head Centre for Engineering Education Research Faculty of Engineering and Built Environment, ⁴Director of Solar Energy Research Institute, Universiti Kebangsaan Malaysia 43600, Bangi, Selangor MALAYSIA Corresponding author: nowshad@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, a conventional structure of CdTe thin film solar cells [1] was investigated and conversion efficiency as high as 13.2% was achieved with the CdTe baseline structure of SnO2/CdS/CdTe. To explore the possibility of ultra thin and high efficiency CdS/CdTe solar cells, the CdTe absorber layer and CdS window layer were decreased to the extreme limit and 1 μ m thin CdTe layer is found to show reasonable range of efficiency with stability. 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 together with the insertion of zinc oxide (ZnO) or zinc stannate (Zn2SnO4) as the buffer layer to prevent forward leakage current. All the simulations 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 μ m-CdTe absorber layer, 60 nm-CdS window layer and 100 nm of ZnO or Zn2SnO4 buffer layer. Furthermore, 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 photovoltaics, high efficiency, CdTe, CdS, zinc oxide, zinc stannate, AMPS 1D

1 Introduction

Thin-film polycrystalline CdTe based solar cells are one of the most promising candidates for photovoltaic energy conversion because of their potential to realize low cost, high efficiency, reliable and stable thin film solar cell. 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 sputtering. Third, CdTe has a high absorption coefficient over 5×105 /cm, which means that all the incident photons with energy greater than the bandgap can be absorbed within the first few microns of thickness 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 thickness required for an absorption layer makes the cost of material for CdTe solar cells relatively 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 reduce the recombination loss as well as lower production time, and the energy needed to produce the solar cells. 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 usage.

efficiencies conversion of However, homojunction CdTe solar cells have not shown encouraging results. Thus, heterojunction cell structure with wide band-gap n-type semiconductor (commonly CdS) and p-CdTe are widely used. Moreover, from optoelectronic and chemical properties, CdS is the best suited n-type heterojunction partner to CdTe for high-efficiency and low-cost cells. The maximum theoretical efficiency for CdTe 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 champion 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 practical CdTe devices with 18–19% that 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 (Voc) then its counterparts. The largest contribution to the efficiency difference with the same bandgap material like GaAs is the Voc, 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 was 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 further be compromised by higher carrier density (~1016 cm-3) and higher absorber lifetime (more than 1 ns) as well as by reducing the significant back-contact barrier height. The strategies for improving voltage and cell performance have been explored utilizing AMPS 1D simulator and have also been thoroughly discussed in this work.

2 Device Modeling and Simulation

Fig. 1 illustrates the conventional 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 laver. Thus, the front contact consists of TCO and a buffer layer. The doping concentration (~1014 cm-3) used in the baseline case has been changed to (~1015 cm-3) more effective and today's practically achievable values for higher efficiency. Considering the low cost feature, silver (Ag) is used as back contact material with back contact barrier height (ΦbL) of 1.25 eV in the modified structured cell instead of Au ($\Phi bL= 0.4 \text{ eV}$). Solar cell simulation could be useful for time saving and cost consumption [6]. In this work, AMPS 1D simulator 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 [7].



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

	n-ZnO/ n-Zn ₂ SnO ₄	n-CdS	$p-CdS_x Te_{1-x}$	p-CdTe
Thickness, W (µm)	0.02-0.5	0.02-0.5	0.0-0.5	0.1-10
Dielectric ratio, ε/ε _o	9.0	9.0	9.4	9.4
Electron mobility, μ_n (cm ² /Vs)	32	350	500	500
Hole mobility, μ_p (cm ² /Vs)	3	50	60	60
Carrier concentration, n/p (cm ⁻³)	10 ¹⁹	10 ¹⁸	10 ¹⁴	5×10 ¹⁵
Bandgap, E _g (eV)	3.35	2.42	1.41	1.45
Density of states, N _C (cm ⁻³)	2.2×10^{18}	2.2×10 ¹⁸	7.5×10 ¹⁷	7.5×10 ¹⁷
Density of states, N _V (cm ⁻³)	1.8×10 ¹⁹	1.8×10 ¹⁹	1.8×10 ¹⁹	1.8×10 ¹⁹
Electron affinity, χ (eV)	4.50	4.50	4.28	4.28

Table 1: Material parameters those have been used in this CdS/CdTe solar cell simulation.

Four basic layers that have been emphasized in this modeling are the buffer layer (Zn_2SnO_4) , n-CdS layer, p-CdS_xTe_{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 cases, reasonable estimations.

In this analysis, the CdTe layer thickness from 10 μ m to 10 nm, CdS window layer thickness from 20 nm to 500 nm and ZnO and Zn₂SnO₄ buffer layer thickness from 10 nm to 500 nm has been varied by keeping all other parameters at the fixed values as shown in Table 1 aiming to achieve the efficient and thinner CdS/CdTe solar cell.

3 Results and Discussion

Numerical modeling techniques can help the understanding of solar cells, and should give the additional ideas to vary structures and cell parameters to improve the cell performance. The number of parameters that can be varied in the particular solar-cell model is larger than 50 [8]. Obviously, a problem with 50 variables is too ambiguous to solve reliably. It is therefore necessary to minimize the number of variable parameters by fixing many of them at "reasonable" values. It was a tough challenge to choose the appropriate parameters. Many of them depend on fabrication techniques and deposition methods and can thus vary among devices. A three-layer device model of a SnO₂/CdS/CdTe solar cell is the starting point for the calculations in this work. A baseline case was utilized to approximate the highest-efficiency CdS/CdTe solar cells at that time, and it was slightly modified to explore the possibility of efficient thinner cells. In this work, first of all the conventional CdTe baseline structure (SnO₂/CdS/CdTe) [1] has been investigated and a conversion efficiency of 13.2% (Voc = 0.85 V, Jsc = 26.8 mA/cm², FF = 0.63) was found 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, $Jsc = 25.76 \text{ mA/cm}^2$, FF = 0.71) with the new CdTe doping concentration (5×10^{15}) 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 1-2 µm [4, 11]. However, to date almost all the high efficiency CdTe solar cells have been fabricated with more than 5 μ m 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 μ m to 6 μ m to explore thinner absorber layer and the results obtained from the 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 μ m. The short circuit current density (*Jsc*) slowly decreased but the *Voc* and *FF* remained unaffected by the reduction of CdTe thickness until 1 μ m, but below 1 μ m of CdTe thickness all the cell output parameters decreased drastically, which has shown good agreement with similar works [9]. As a result, the efficiency showed very slow decreasing trend with the reduction of CdTe thickness until 1 µm and below 1 µm of CdTe thickness decreases rapidly which indicates that 1 µm thick CdTe cell has possibilities with very small decrease or loss in efficiency. A conversion efficiency of 14.6% (Voc = 0.92 V, Jsc = 24.6 mA/cm², FF = 0.706) has been achieved for 1 μ m thick CdTe cell, which indicates that with only 25% CdTe absorber material of the baseline cell the compromise for efficiency is only 0.8% (15.4% to 14.6%). These results are in good agreement with related published results by others on CdTe cells [10].







Fig. 3: Effect of CdTe thickness on the quantum efficiency.

The spectral response of the above CdTe baseline case cell (SnO₂/CdS/CdTe) with different CdTe layer thickness from quantum efficiency (QE) calculation by AMPS 1D is shown in Fig. 3. It is evident that the spectral response starts decreasing at the operating wavelength of 460 nm until 820 nm with decreases of the CdTe layer thickness. It also indicates that the thicker CdTe layer has shown higher QE that implies that the conversion efficiency will be higher but require more CdTe materials. Thickness reduction of the CdTe absorber layers would not only be useful to minimize the material cost in the production process but could also lead to better solar cell properties by reducing recombination losses in the bulk [10, 11]. However, thin films which are compact and free of pinholes, control of the film growth and recrystallization due to post-deposition treatment is necessary to obtain. The latter are known to be critically affected e.g. by the type and structure of the front contact material [12] or the deposition temperature [13]. Employing the CSS technique, CdTe films can be deposited at high rates and with a good film quality while the material yield is very high. CSS-CdTe films can consist of large grains being useful for the electronic transport properties. However, the actual film thickness needed may be larger than the absorption depth due to the possibility of increased shunting in

thinner films. Thus considering all these the CdTe layer thickness was selected at 1 μ m for this investigation, however there are possibilities 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.

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 developed during the CSS film growth process). The CdS_xTe_{1-x} layer thickness depends on CSS growth time which can be reduced in the 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 the simulation are shown in Fig. 4.

It can be observed from Fig. 4 that the solar cell output parameters are strongly dependent on CdS_xTe_{1-x} thicknesses below 70 nm but above 100 nm it is not much affected. In order to overcome the fabrication challenges, the CdS_xTe_{1-x} layer thickness was selected to 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 is mainly due to the improvement of *Voc* and FF but with a minimum sacrifice in Jsc.



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

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 consequently the efficiency. Fig. 5 shows the effects in details of CdS layer reduction from 200 nm to 20 nm on the cell parameters such as *Jsc*, *Voc*, *FF* and η from AMPS 1D simulation, with CdTe layer thickness of 1 µm and CdS_xTe_{1-x} layer thickness of 10 nm.

Fig. 5 shows that *Jsc* has improved greatly with reduced CdS layer with no effect on *Voc* and a little decrease in *FF*. As a result, η increased with reduced CdS layer. The QE of CdS layer thickness variation from 20 nm to 300 nm is shown in Fig. 6.

As can be seen, when the wavelength is below 510 nm the quantum efficiency is much affected with the increasing CdS layer thickness and finally the conversion efficiency. These results are in good agreements with other literatures [14]. However, to date, it is impractical to fabricate good quality devices with CdS film thickness below 50 nm by CBD process that has been 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 is mainly due to the improvement in *Jsc*.



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



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 may allow forward leakage current to front contact through possible pinholes 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 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. The modified structure consists 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 a very thin resistive buffer layer, the CdS layer thickness can be reduced to 50 nm, which significantly improves the blue response, CdS film morphology and conversion efficiency of the CdTe devices [15]. 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

have been tried in this work. Doped ZnO showed promising results to be implemented in thin film solar cells [16] and $Zn2SO_4$ was used as a buffer layer in the height efficiency CdS/CdTe solar cell [4]. The ZnO or Zn_2SO_4 as a buffer layers have 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 I-V characteristics obtained by AMPS are shown in Figure 7.

The ZnO insertion shows almost the same results as with Zn₂SO₄ insertion. The simulation also shows that the solar cell output characteristics are independent of ZnO or Zn₂SO₄ thicknesses 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 1.4% efficiency has come from 0.9 mA/cm^2 gain in *Jsc* than without the buffer layer. Fig. 8 shows the band diagram of the finally selected cell configuration of Glass/SnO₂/ZnO/CdS/CdTe/Ag with illumination at 0 V to investigate the band diagram.



Fig. 7: Effect of ZnO and Zn_2SO_4 on the solar cell I-V characteristics.



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/SnO₂/ZnO/CdS/CdTe/Ag with illumination at 0 V to investigate the performance. It is clear 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 (Zn₂SnO₄)/CdS and CdS/CdTe. ZnO insertion produced larger spike than Zn₂SnO₄ insertion showing 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 the final cell conversion efficiency with operating temperature ranged from 25°C to 100°C as shown in Fig. 10. It is evident from Fig. 10 that the conversion efficiency linearly decreases with the increase of operating temperature at a temperature coefficient (TC) of -0.4%/°C, which also indicates the degree of stability of the cell at higher operating temperature or in stressed conditions. This result is in good agreement with related works [17].



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

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. Open circuit voltage (Voc) and fill factor (FF) increased to 150 mV and 14%, respectively with a Jsc decrease of 0.65 mA/cm² compared to 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 (SnO₂/CdS/CdTe) of 4 µm thick CdTe. Moreover, a potential idea was found to increase the cell efficiency by reducing CdS window layer thickness along with suitable buffer layer insertion. 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 spectral response of the cell at the blue region. The Zn₂SO₄ buffer layer insertion showed almost the same results with ZnO insertion. Furthermore, the result of cell operating temperature has shown the stability to some extent of this cell at higher operating temperatures with a temperature coefficient (TC) of -0.4%/°C. Therefore, it is suggested that efficient and cost-effective ultra-thin film CdS/CdTe solar cell can be realized with 60 nm of CdS layer, 1 μ m of CdTe layer and 100 nm of ZnO/Zn₂SO₄ buffer layer.

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