ASSESSING THE EFFECTS AND IMPACTS OF THE CdSTe INTERLAYER IN THE PERFORMANCE OF THE CdTe-CdS THIN FILM SOLAR CELLS THROUGH SIMULATIONS

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ABSTRACT
CdTe based solar cells have proved to be the most successful thin film PV solar cells with their full industrial production. However, the needed improvement in output efficiency of these cells is constrained by major issues such the poor understanding of the ternary CdS_xTe_{1-x} interlayer, formed at the CdS-CdTe interface. While it is believed to have both beneficial and negative effects on the cell performance, its exact mechanism and extent are not fully explored. In this work, the AMPS-1D software was used to model this interlayer, using several of its variables such as thickness, bandgap as well as the thickness of the bounding CdS layer. Results show that the interlayer thickness reduces cell performance, through Jsc, Voc, FF and J-V curves, with best efficiencies of 17.892% ($Jsc=27.043 mA/cm^3$, $Voc=0.871V$, FF=0.8) obtained at zero thickness, falling down by nearly 20% at CdS_xT_{1-x} thickness of 100nm. As the bandgap is varied, maximum cell performance of 17.85% ($Jsc=27.76$, $Voc=0.91V$ and FF=0.81) was found at 1.7eV. Similarly, increasing CdS thickness also reduced cell performance, by reducing the quantum efficiency. The results indicate that if the CdS_xTe_{1-x} layer has a thickness of up to 100nm, and a bandgap of around 1.7eV, then cell efficiencies of around 18% were feasible even for ultra-thin CdTe layers of 1μm.

Keywords: CdS_xTe_{1-x}, optical absorption, efficiency, pinhole.

INTRODUCTION
The search for a viable photovoltaic solar cell technology that can compete favorably with conventional fossil fuels has recognized CdTe based thin film solar cells as a viable pathway to achieve the required low-cost photovoltaic device. This is because of the numerous material and manufacturing advantages of CdTe material. Chief amongst these are its high optical absorption coefficient, near ideal bandgap (1.5eV) for solar spectrum absorption and multiple, low-cost fabrication methods. (Mathew, et al. 1999, Enriquez,2004; Hernandez et al. 2006 and Romeo et al 2007). From optical, electronic and chemical properties, CdS is considered the best suited n-type hetero-junction partner to CdTe for high efficiency and low cost PV (Poortmans and Arkhipov 2006) with a maximum theoretical efficiency of about 29% for such cells (Tyan and Perez 1982). On the industrial scale, CdTe solar cells are considered the most successful thin film solar cells with First Solar, being the first PV solar cell manufacturer to reach an annual production capacity of over 1GW, in 2009 and at an equally lowest production cost of 76c/Wp in 2010, and with a production projection of 2.1 GW in 2012. Its NREL-measured module efficiency is up to 12.5%. (First Solar 2024; First Solar 2011 and Cadmium Telluride Photovoltaics 2011). These CdTe-based PV devices have achieved 22.1% efficiency and have captured ~5% of the current world PV market (Gorai, 2023 and Jayswal 2024) with more than 30 GW peak (GWp) generating capacity (Scarpulla , 2023)

Despite the successes of these cells however, there are still outstanding issues for achieving better performance and cheaper device. Among these is the creation of the CdS_xTe_{1-x} interlayer formed at the P-N junction of the CdS/CdTe layers, as a result of S and Te interdiffusion, caused by the high temperature fabrication process. It is generally accepted that for higher cell performances, the CdCl2 activation treatment and annealing at $380-500^oC$ is necessary for CdTe solar cells. This process makes CdS and CdTe recrystallize, leading to the formation of the CdS_xTe_{1-x} interlayer, due to the inter-diffusion of S and Te across the boundary. Although it is believed that this layer has both beneficial and negative effects, its exact formation and effects on the solar cell is poorly understood.

However, the following are believed to be its beneficial effects:
- ➤ dopes p-CdTe
- ➤ increased grain growth
- ➤ passivation of the grain boundaries
- ➤ reduction of strain across the CdS/CdTe interface created by the lattice mismatch'
- ➤ recrystallization (Matulionis 2002 and Romeo 2002)

The band bowing effect, shown in Fig. 1, can shift the cell response to the blue or red region, depending on the layer bandgap (Dhere 1997and Matulionis 2002).
Gonzalezuse et al (2009) used a theoretical method for the determination of the interface charge density in the CdS /ternary/CdTe heterojunction and the band discontinuity ΔE_V simultaneously.

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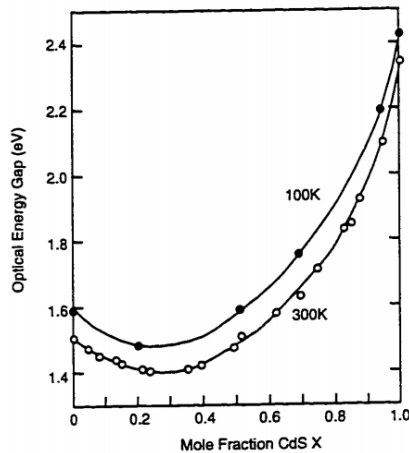
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Figure 1. Energy Bandgap of CdSxTex-1 [10]

In addition, the quantum efficiency of the solar cell is affected by the thicknesses of both CdS and CdTe layers (Dhere, 1997) with serious implication in the ultra-thin solar cells, where very thin layers (CdS<60nm, CdTe<1μm) are involved. Although oxygenated (CdS:O) have been reported to reduce some of the problems of CdS_xTe_{1-x} (Wu et al. 2002 and Amin et al 2010), but other problems arise, such as lower adhesion and thus higher series resistance, eventually, leading to some loss of cell efficiency. Thus, it becomes imperative that better understanding of this interlayer is explored and exploited with the aim of predicting and utilizing its exact behaviors for better performing CdTe thin film solar cells.

This work proposes the investigation of the effects of these important variables (bandgap and thickness of CdS_xTe_{1-x} and thicknesses of CdS) in order to understand their relationships and effects on solar cells as well as explain the observed behaviors. The popular AMPS-1D software has been used to model and simulate the different cell structures and assess their performances. The cell output variables considered are Jsc, Voc, FF, efficiency, J-V and QE.

MODELING AND SIMULATIONS
The baseline CdTe solar cell structure, as shown in Fig. 2, was chosen to investigate the impact of the CdS_xTe_{1-x} interlayer. This glass-based, superstrate structured cell consists of a fluorine doped tin oxide (SnO_2:F) as transparent conducting oxide (TCO), cadmium sulphide (CdS) as window layer and cadmium telluride (CdTe) as the absorber. A metallic back contact of copper/gold (Cu/Au) is selected in order to produce acceptable Ohmic back contact. Numerical modeling, simulation and analysis of the structure, performance and understanding the physics of solar cells and other photonic systems has been a useful means of gaining relevant insight into the possible behavior of such structures in real life situations. The AMPS-1D program has been developed to realistically simulate the electrical and optical characteristics of the thin film solar cells (Matulionis, 2023). However, the successful applications of this program requires the user to input appropriate and practically realistic material parameters for the structures. In this study, these parameters have been obtained from results of experiments, literature, established theory and reasonable estimates. The material properties used in this work are presented

in Table 1. In previous simulation studies on CdS_xTe_{1-x} layer, the assigned material properties, such as bandgap, dielectric permittivity, type and concentration of carriers, and electron affinity, were given fixed values throughout the simulation. In this work, these values are assumed to vary, depending on the value of x in the CdS_xTe_{1-x} ternary. Thus, as the bandgap changes from lower value, the material properties were given values closer to that of CdTe, while at the higher end, they approach those of CdS.

Table 1:
Material parameters used in simulation.

Parameter	SnO_2	CdS	CdS_xTe_{1-x}	CdTe
W (μm)	0.01- 0.5	0.025- 0.2	0.0-0.10	0.1- 6.0
$\varepsilon/\varepsilon_o$	9.0	10.0	9.4-10.0	9.4
μ_c (cm^2/Vs)	100	100	100-320	320
μ_p (cm^2/Vs)	25	25	25-40	40
n, p (cm^{-3})	10^{17}	10^{17}	$5\times10^{15}/10^{17}$	5×10^{15}
E_g (eV)	3.6	2.42	1.4-2.4	1.45
N_C (cm^{-3})	2.2×10^{18}	2.2×10^{18}	8.0×10^{17}	8.0×10^{17}
N_V (cm^{-3})	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}
χ (eV)	4.50	4.50	4.28-4.5	4.28

RESULTS AND DISCUSSION
The results of the simulations are presented and analyzed by considering the output parameters' variation with different input variables, including thickness of each layer, and CdS_xTe_{1-x} bandgap. Variation of the CdS_xTe_{1-x} layer thickness are presented in Figs. 3 to 6, showing its effects on Jsc, Voc, FF and efficiency. It is obvious that as the layer thickness increases, all the cell performance parameters reduce, as is commonly believed. The increased thickness reduces optical transmission, at the same time increases bulk resistance, thus higher series resistance. In addition, the defects densities in this interlayer increases, leading to higher recombination rates. These effects lead to lower Jsc, in first case and smaller Voc and FF in the later. There is overall fall in efficiency, as illustrated by the J-V curves. These results can be explained further from the curves of the electric field and quantum efficiency of the cells. The field across the junction indicates that thinner layer produces stronger fields, thus higher possibility of carrier collection. This ultimately helps increase Voc. Similarly, the quantum efficiency is better for thinner CdS_xTe_{1-x}, resulting in higher Jsc. Next, the bandgap was varied and its effect on cell performance was investigated. It was found, as presented in Figure 7, which all the parameters (Jsc, Voc, FF and η) attain their maximum around 1.7eV, which, according to Fig.1, correspond to an x value of 0.75.
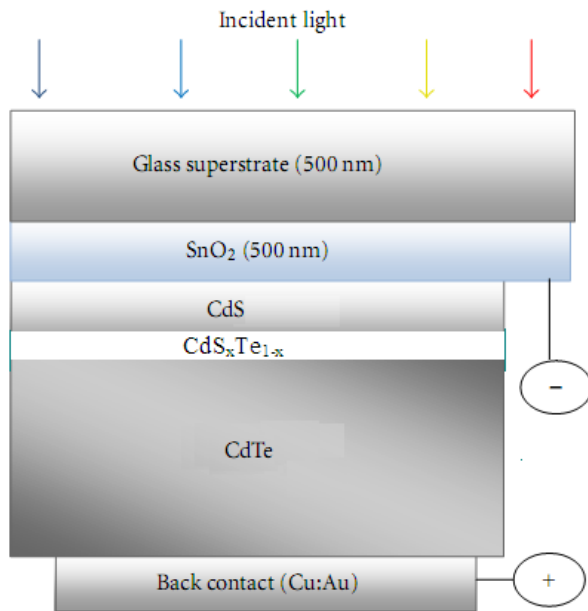
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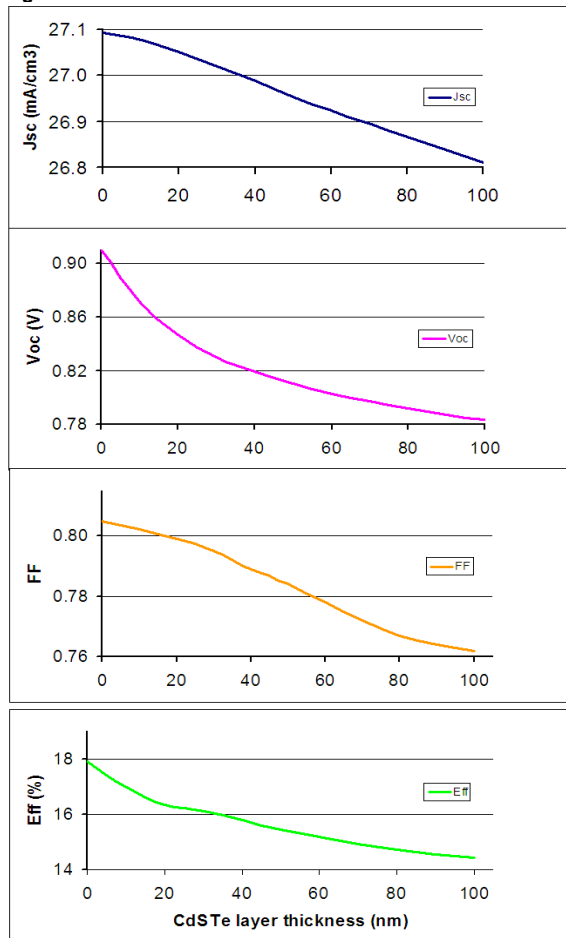**Figure 2**. CdTe Solar Cell Model

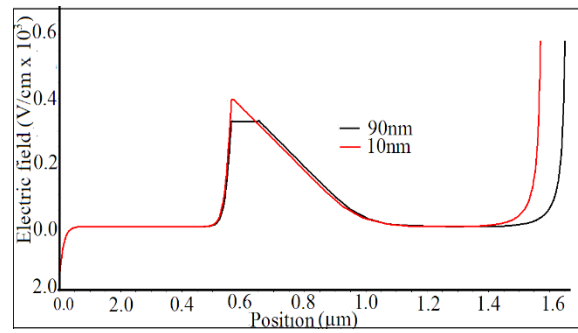**Figure 3**. Effects of CdS$_x$Te$_{1-x}$ layer on cell performance

Figure 4 The electric field of two CdS$_x$Te$_{1-x}$ layers thickness
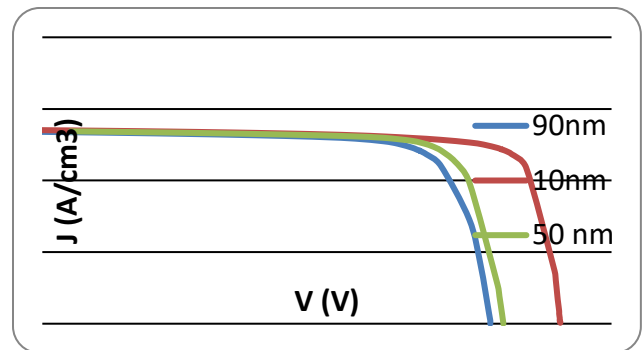

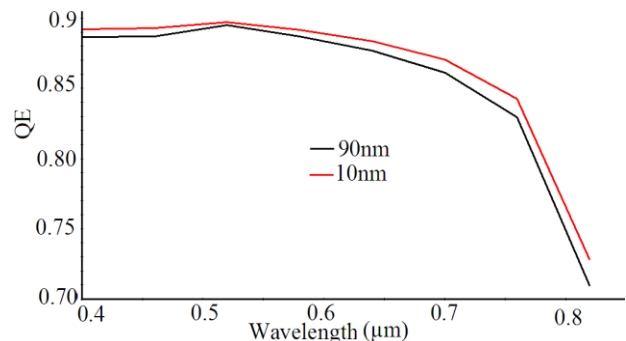**Figure 5**. J-V Characteristics dependence on CdS$_x$Te$_{1-x}$ thickness

Figure 6. Effect of CdS$_x$Te$_{1-x}$ thickness on QE

This obviously implies that best cell performances are most likely obtained when the interlayer gap comes near this value. However, the value of Eg is not exactly predictable, thus attempts should be made, during fabrication, to obtain higher value of Eg. The JV curve and QE, presented in Fig. 8 and Fig. 9, show the impact of bandgap on the cell, supporting this, where best results are obtained at band gap of 1.7eV. By using this optimized band gap, the effects of the CdS window layer thickness is also investigated, in order to understand its effects on the cell. The significance of this is that recent efforts towards improving cell performance has concentrated efforts in reducing the CdS thickness, in order to reduce optical absorption, thereby improving Jsc, at same time reduce material and energy input, thus cheaper cost (Amin et al 2000). These are presented in Figure 9.
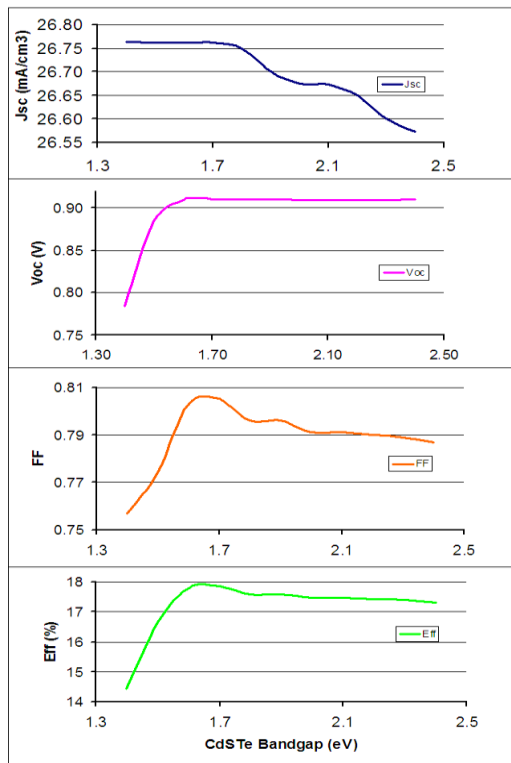
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Figure 7. Effects of CdS$_x$Te$_{1-x}$ Bandgap on cell performance
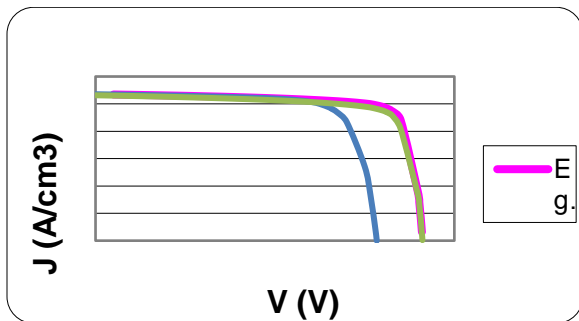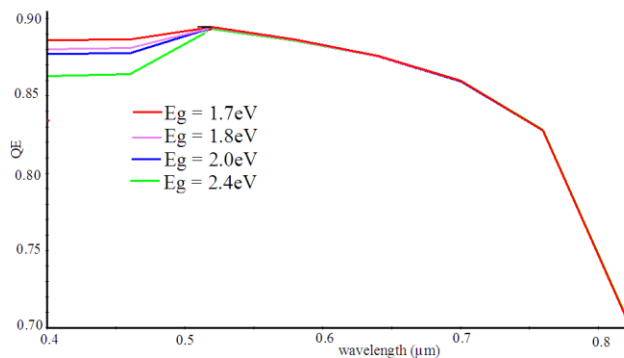

Figure 8. Impact of bandgap on JV curves

Figure 9. Quantum Efficiency of different CdSTe bandgap

Thicker CdS layer reduces Jsc, FF and eventually, efficiency, while Voc appears unaffected. It is known that CdS thickness reduces the photon reaching the absorber layer, thus reduced electron-hole pair generation and so lower Jsc (Amin et al 2010). The lower fill factor may be due to higher series resistance from the thicker CdS, as well as possible poor mix in the CdSTe layer (Amin et al 2000). However, the general agreement amongst researchers is that a value of 50-80nm will give optimum performance, with the insertion of a buffer layer between the TCO and this window layer (Hodges, 2009). This is because thinner CdS layers are difficult to fabricate without producing pinholes, causing the front contact and absorber layer to shunt, thereby shorting the cell. However, by introducing the high resistive thin layer (HRL) between TCO and CdS, this effect is eliminated.
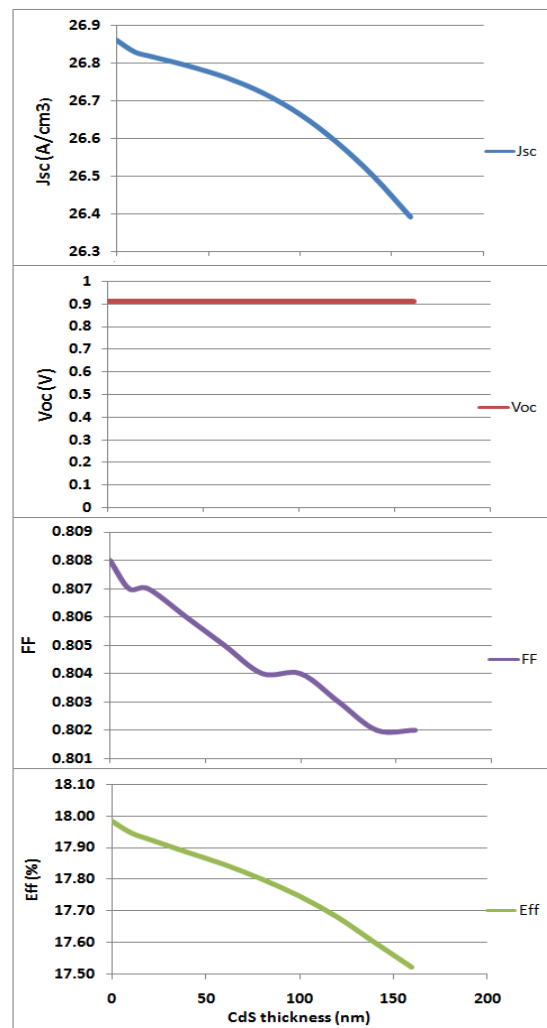

Figure 10. Effect of CdS thickness on cell performance

Conclusion

The CdS$_x$Te$_{1-x}$ interlayer has been modeled and simulated using AMPS 1-D, by varying its thickness, bandgap as well as thicknesses of adjacent CdS window layer in order to understand their effects in CdTe solar cells. The results show that thinner

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(CdS$_x$Te$_{1-x}$ and CdS) layers give better performance due to increased optical transmission, lower defect state, higher quantum efficiency and better carrier collection. An optimal bandgap of 1.7eV was found to produce best cell efficiency of 17.85%, at which all cell parameters improved. Similarly, the results show that thicker CdS window layer will lead to reduced Jsc, FF and efficiency. Thus, the performance of CdTe solar cells can be better understood and fabrication processes adjusted to obtain better performing solar cells.

Acknowledgements

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