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Numerical Simulation of Prospective Buffer Layers in Cadmium Telluride (CdTe) Thin Film Solar Cells

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ABSTRACT

This study aims to enhance the performance of cadmium telluride (CdTe) thin film solar cells through a comprehensive investigation of various buffer layer materials and their influence on device efficiency. Utilizing the SCAPS-1D simulation tool, initially a baseline model has been established for the CdTe solar cell, characterized by a 5 µm thick CdTe absorber layer, a 25 nm thick CdS buffer layer, and carrier concentrations of 10^{17} cm^{-3} for CdTe and 10^{18} cm^{-3} for CdS. This baseline configuration yielded key photovoltaic parameters: open-circuit voltage (Voc) of 1.0686 V, short-circuit current density (Jsc) of 23.8378 mA/cm^2, fill factor (FF) of 88.13%, and an overall efficiency (η) of 22.45%. Building upon this, various buffer layers, including materials such as MZO (magnesium zinc oxide), were introduced to evaluate their impact on device performance. Results indicated that the incorporation of MZO, particularly when used without the traditional CdS layer, significantly enhanced the photovoltaic parameters, achieving an efficiency of 23.66%. Additionally, the MZO buffer layer contributed to improved device stability under elevated temperature conditions and in the presence of structural defects, indicating superior robustness compared to conventional buffer configurations. These findings suggest that optimizing buffer layer materials, especially using MZO, can lead to notable improvements in the efficiency of CdTe solar cells. In conclusion, this research provides valuable insights into material selection and device architecture, paving the way for the development of more efficient thin film photovoltaic technologies.

Keywords: CdTe thin film solar cell; buffer layer; thickness; carrier concentration; Scaps 1-D.

INTRODUCTION

Solar energy is a renewable and environmentally friendly resource that offers a sustainable alternative to conventional fossil fuels. Among various solar technologies, photovoltaic (PV) cells, particularly Cadmium Telluride (CdTe) solar cells stand out due to their high efficiency and cost-effectiveness in thin-film applications (Turgeon & Morse 2023). The fundamental operation of a solar cell involves the absorption of sunlight, which excites electrons within the semiconductor material, creating electron-hole pairs. The separation and collection of these charge carriers, facilitated by the p-n junction, generate electrical energy (Anon 2020; Pukala 2023).

The development of buffer layers in CdTe solar cells has been pivotal in enhancing device performance. Historically, the inclusion of buffer layers was first proposed to address issues such as interface recombination, poor charge extraction, and stability concerns at the heterojunction interface. The buffer layer is placed between the CdS layer and the TCO (Transparent Conductive Oxide) layer. The main function of the buffer layer is to optimize the interface between the CdS window layer and the TCO, ensuring efficient movement and collection of charge carriers while reducing recombination losses. A crucial characteristic of the buffer layer is its electrical conductivity. When the TCO layer in contact with the CdS is highly resistive or nearly insulating, it helps prevent electrons from getting trapped and improves the overall performance of the solar cell (Von Roedern, 2001). This setup helps maintain a high V_{OC} and enables more efficient charge extraction, leading to higher efficiency. The buffer layer enhances the long-term stability and reliability of CdTe solar cells. Early research demonstrated that inserting a buffer layer between the CdS window layer and the TCO layer could significantly improve the electrical contact quality and suppress defect states that act as recombination centers (Ali et al. 2025; Git et al. 2024; Hafaifa et al. 2024; Lii et al. 2024; Sarra et al. 2024). In summary, the buffer layer is essential for optimizing the interface between the CdS window layer and the TCO, improving charge transport, reducing recombination losses, and enhancing the overall stability and performance of CdTe thin film solar cells.

This study aims to build upon this foundation by investigating the role of different buffer layer configurations in CdTe solar cells. Using SCAPS-1D simulation software, we analyze how various buffer materials and setups influence electrical parameters, especially in the presence of defects and temperature variations. Our goal is to identify optimal buffer layer conditions that enhance efficiency, stability, and overall device performance.

METHODOLOGY

MODELLING

There are four key parameters in solar cells, which are V_{OC}, J_{SC}, FF, and η. V_{OC} is the maximum voltage a solar cell can produce when no current is flowing. J_{SC} is the highest current that the cell can generate, measured when the voltage is zero. FF indicates how efficiently the cell converts light into energy, calculated by dividing the cell's maximum power output by the product of V_{OC} and J_{SC}. Lastly, η represents the overall efficiency of the solar cell, showing the percentage of incoming light converted into electrical energy. It is calculated by comparing the cell's maximum power output to the power of the incident light.

The methodology is divided into four phases, as shown in Figure 1. First, we conduct a literature review to identify factors affecting solar cell efficiency and gather data on buffer layers, defects, and temperature effects. Then, we use the SCAPS-1D simulator to optimize the CdTe absorber and CdS window layers by varying their thickness and carrier concentration. In the second phase, we simulate the impact of different buffer layers, adjusting their thickness and carrier concentration, and assess their performance with and without the CdS layer. The third phase involves defect analysis of the CdTe baseline and buffer layer structures. Finally, we analyze the effect of temperature on these structures to determine their resilience. This comprehensive approach aims to enhance the overall efficiency and stability of CdTe thin film solar cells.

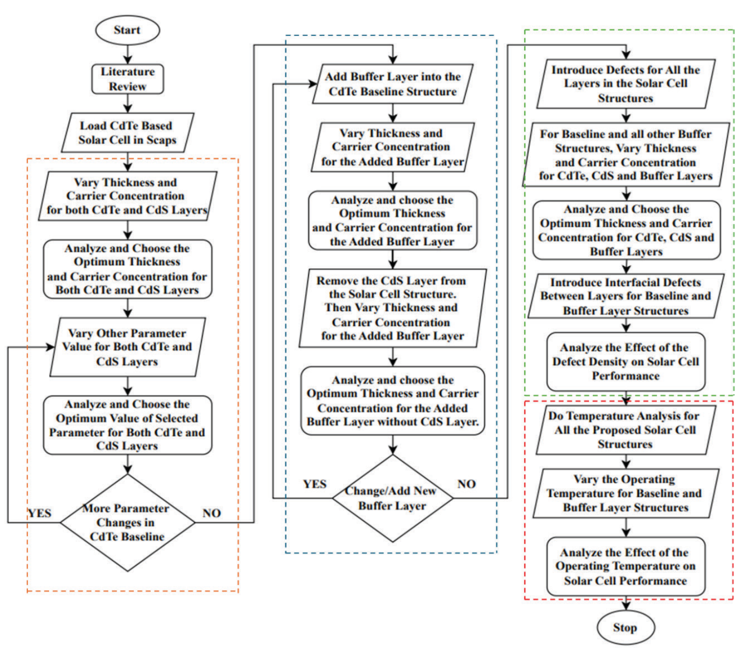

FIGURE 1. Flowchart of the study

PARAMETER OF SOLAR CELL

This study consists a baseline and buffer layer structure model for CdTe solar cell as shown in Figure 2 (Rassol et al. 2021; Bhari et al. 2023; Doroody et al. 2023; Ibrahim et al. 2022) and the parameters of the CdTe solar cell such as bandgap, electron affinity, hole concentration, hole mobility and thickness for the layers as shown in Table 1 (Ali et al. 2025; Bhari et al. 2023; Doroody et al. 2023; Rassol et al. 2021; Taoufik et al. 2022). The defect parameters for the layers in the solar cell is shown in Table 2 (Bhari et al. 2023). Figure 3 shows the design interface of CdTe solar cell using SCAPS-1D simulator.

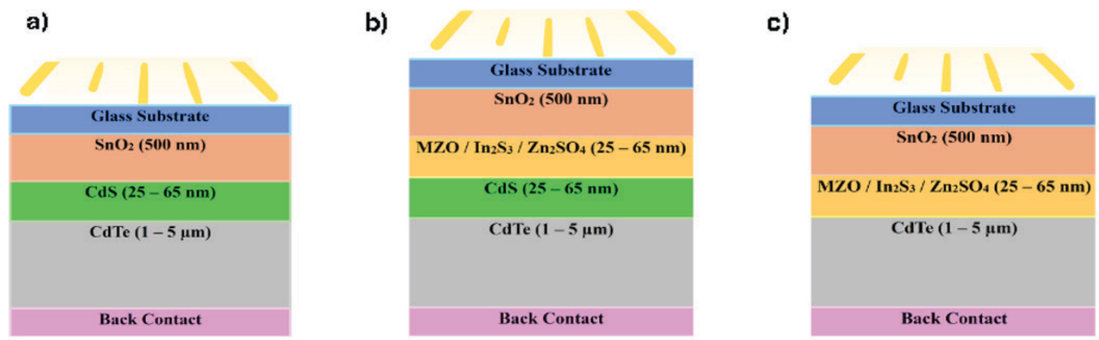

FIGURE 2. CdTe solar cell structure a) baseline, b) buffer layer with CdS and c) buffer layer without CdS

TABLE 1. Simulation parameters used in this study

Parameter	SnO_2	CdS	CdTe	MZO	In_2S_3	Zn_2SO_4
Thickness (nm)	500	25 – 65	1000 – 5000	25 – 65	25 – 65	25 – 65
Bandgap (eV)	3.6	2.4	1.5	3.5	2.8	3.5
Electron Affinity (eV)	4.0	4.0	3.9	4.45	4.3	4.0
Dielectric Permittivity	9.0	10.0	9.4	10	13.5	9
CB Effective Density (cm^{-3})	2.2×10^{18}	2.2×10^{18}	8.0×10^{17}	2.0×10^{17}	1.8×10^{19}	2.2×10^{18}
VB Effective Density (cm^{-3})	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	4.0×10^{18}	1.8×10^{19}
Electron Thermal Velocity (cm/s)	10^7	10^7	10^7	10^7	10^7	10^7
Hole Thermal Velocity (cm/s)	10^7	10^7	10^7	10^7	10^7	10^7
Electron Mobility (cm^2/Vs)	100	100	320	100	400	100
Hole Mobility (cm^2/Vs)	25	25	40	10	21	25
Uniform Donor Density N_D (cm^{-3})	10^{17}	$10^{14} – 10^{18}$	0	$10^{14} – 10^{18}$	$10^{14} – 10^{18}$	$10^{14} – 10^{18}$
Uniform Acceptor Density N_A (cm^{-3})	0	0	$10^{13} – 10^{17}$	0	0	0

TABLE 2. Defect Parameters

Parameter	Buffer Layers	CdS/CdTe
Type of defect	Neutral	Neutral
E_t (eV) above E_V	0.6	0.8
Cross section Area of electron (cm^2)	10^{-15}	10^{-15}
Cross section Area of hole (cm^2)	10^{-15}	10^{-15}
N_t (cm^{-3})	10^{13} - 10^{18}	10^{13} - 10^{18}

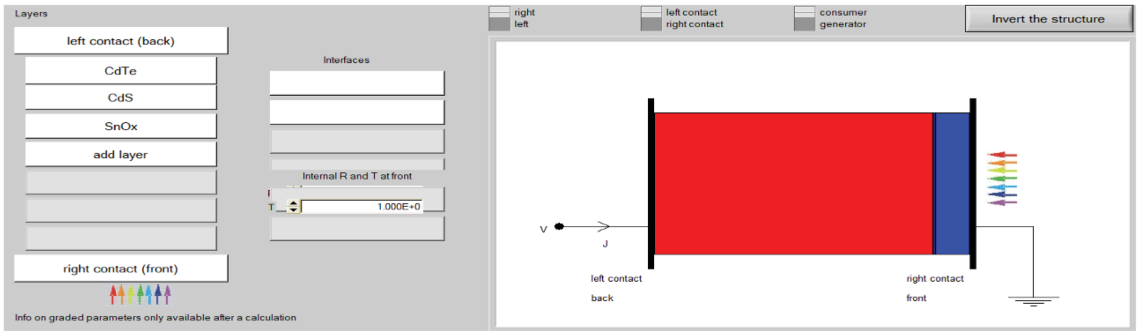

FIGURE 3. CdTe base design using SCAPS-1D

RESULTS AND DISCUSSION

CDTE LAYER OPTIMIZATION

The optimization of the baseline CdTe structure with CdS, variations in the CdTe layer's thickness and carrier concentration have been completed to find the perfect values for a thin film CdTe structure with CdS as a window layer. The thickness and carrier concentration of the CdTe absorber layer were varied from 1000 to 5000 nm and 10^{13} cm^{-3} to 10^{17} cm^{-3}, respectively. As CdTe layer's thickness increases, the values of V_{OC}, J_{SC}, FF, and efficiency (η) also rise, as shown in Figure 4. A thicker CdTe layer absorbs more light, creating more electron-hole pairs, which leads to a higher V_{OC} due to the increased separation of these pairs. This enhanced light absorption generates more charge carriers, resulting in a higher J_{SC}. Additionally, a thicker CdTe layer reduces recombination losses, improving the FF (Parathraju and Umasankar 2025). Overall, the solar cell's efficiency improves with increased CdTe thickness due to better light absorption and conversion to electrical energy.

On the other hand, as the carrier concentration of the CdTe layer rises, V_{OC}, FF, and efficiency also increase, except for J_{SC}, as in Figure 4. Higher carrier concentration means more charges are available to fill recombination gaps, raising V_{OC} (Pepa et al. 2025). However, it also increases recombination rates, which reduces the number of charge carriers collected by the electrodes, thus decreasing J_{SC}. FF improves with higher carrier concentration because it reduces recombination losses. Overall efficiency increases due to reduced recombination at higher carrier concentrations. From the overall results in Figure 4, the optimum thickness and carrier concentration of the CdTe layer are 5000 nm and 10^{17} cm^{-3}, respectively, resulting in V_{OC} = 1.0686 V, J_{SC} = 23.8378 mA, FF = 88.13% and η = 22.45%.

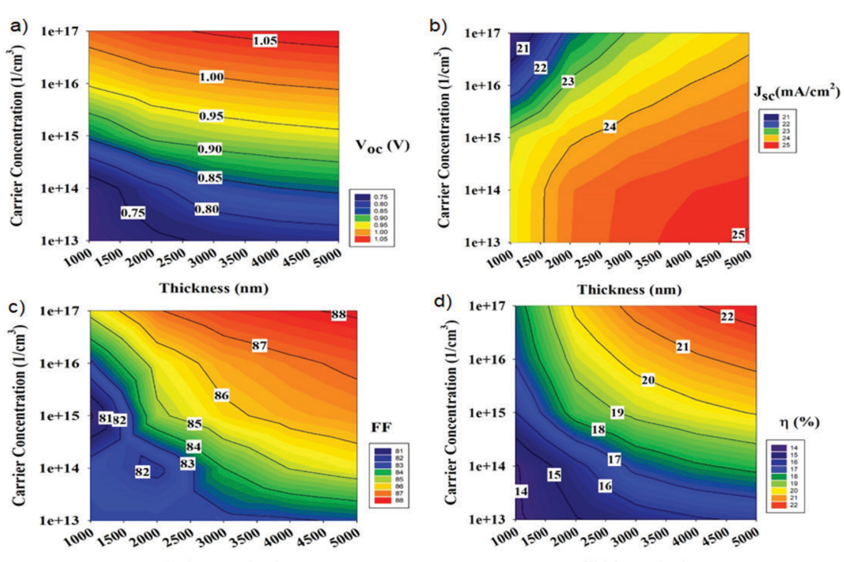

FIGURE 4. Effect of CdTe layer thickness and carrier concentration on solar cell performance

CDS LAYER OPTIMIZATION

The CdS layer in the CdTe baseline solar cell serves as the window layer, which allows light to pass through to the CdTe absorber layer and collect the generated current. The V_{OC} is mainly determined by the properties of the absorber layer and its junction with the CdS layer. So, changing the thickness and carrier concentration of the CdS layer does not affect the V_{OC}. From Figure 5, the variation in the CdS layer's thickness from 25 nm to 65 nm has no impact on J_{SC}, FF or η; this indicates that this range does not influence the light absorption, carrier generation or recombination. However, increasing the CdS layer's carrier concentration from 10^{14} cm^{-3} to 10^{18} cm^{-3} improves the J_{SC}, FF and η. Higher carrier concentrations enhance the conductivity of CdS and boost FF, leading to better overall efficiency. The optimal thickness and carrier concentrations for the CdS layer are 25 nm and 10^{18} cm^{-3}, as shown in Figure 5 and resulting in $V_{OC} = 1.0686$ V, $J_{SC} = 23.8378$ mA, FF = 88.13% and η = 22.45%.

BUFFER LAYER ANALYSIS

The buffer layers were added to the CdTe solar cell, as shown in Figure 2 (b), which is produced using the existing CdTe base solar cell from the previous study, which is already optimized. Then, the CdS layer is removed from the buffer layer structure, as shown in Figure 2 (c), for further study of buffer layer impacts on the performance of solar cells. The buffer layers thickness varied from 25 nm and 65 nm. The carrier concentration varied from 10^{14} cm^{-3} and 10^{18} cm^{-3} for the buffer layers. The thickness and carrier concentration of the buffer layer for both structures with and without the CdS layer is reviewed to determine the highest performance of the CdTe-based solar cells.

For the MZO buffer layer analysis, from Figure 6, as the layer gets thicker, it absorbs more light itself, hindering the J_{SC} because fewer light-generated carriers are available to create current. Fortunately, the FF seems relatively unaffected by MZO thickness, indicating minimal changes in internal resistance or places where generated current might be lost. The downside to a thicker MZO layer is a decrease in overall efficiency due to the reduced J_{SC}. Striking a balance, a thickness of 25 nm seems ideal for both cell configurations with and without CdS. This choice leads to efficiencies of 23.48% for the cell with CdS and 22.66% for the one without CdS. For MZO with CdS structure, the J_{SC} and η increase as the MZO carrier concentration increases from 10^{14} cm^{-3} to 10^{16} cm^{-3}, shown in Figure 6, then decreases further where a higher concentration may introduce recombination centers within the MZO layer, reducing the J_{SC} and η. The FF value does not change with the carrier concentration of MZO. For MZO without CdS structure, the J_{SC}, FF and η all increase as the MZO carrier concentration increases, where this structure benefits from higher concentration for the better overall performance of solar cells. The optimum MZO carrier concentration is 10^{16} cm^{-3} for MZO with CdS structure and 10^{18} cm^{-3} for MZO without CdS, which obtain the optimum efficiency of 22.62% and 22.66%, respectively, as shown in Figure 6.

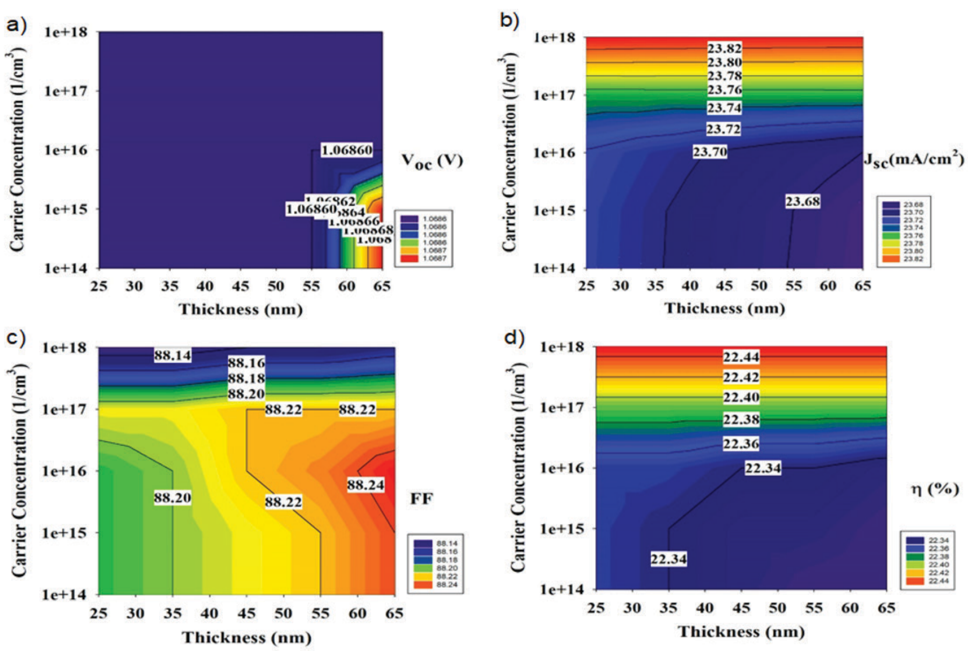

FIGURE 5. Impact of CdS layer thickness and carrier concentration on solar cell performance

For In_2S_3 buffer layer analysis, all the measurement values of V_{OC}, J_{SC}, FF and η of the solar cell for both structures of In_2S_3 remain constant with the changes in the thickness of In_2S_3 as shown in Figure 7. This indicates that within the examined range, the thickness of In_2S_3 does not significantly affect the light absorption, carrier transport, or recombination within the device for the solar cell. Since the thickness of In_2S_3 in both structures does not impact the performance of the solar cell, the optimum thickness of In_2S_3 is chosen as 25 nm and results η of 23.57% and 23.40% for both with and without CdS structure. The J_{SC} and η for In_2S_3 with CdS increase as the carrier concentration increases while FF remains relatively constant. This states that a higher carrier concentration improves the conductivity within the In_2S_3 layer, allowing for better collection of photogenerated current and boosting the overall efficiency. The structure of In_2S_3 without the CdS layer, J_{SC}, FF and η all increase as the carrier concentration of In_2S_3 increases. The absence of the CdS layer makes the solar cell performance more sensitive to In_2S_3 conductivity. Higher In_2S_3 carrier concentration improves conductivity and reduces recombination losses in the solar cell without CdS. When comparing both In_2S_3 structures, In_2S_3 without a CdS layer might absorb more light before reaching the CdTe layer and have some recombination losses within the cells. Thus, its J_{SC} and FF values are lower than In_2S_3 with the CdS layer. The In_2S_3 without a CdS layer structure might lose some energy due to non-ideal band alignment or increased surface recombination, which reduces the overall efficiency of the solar cell.

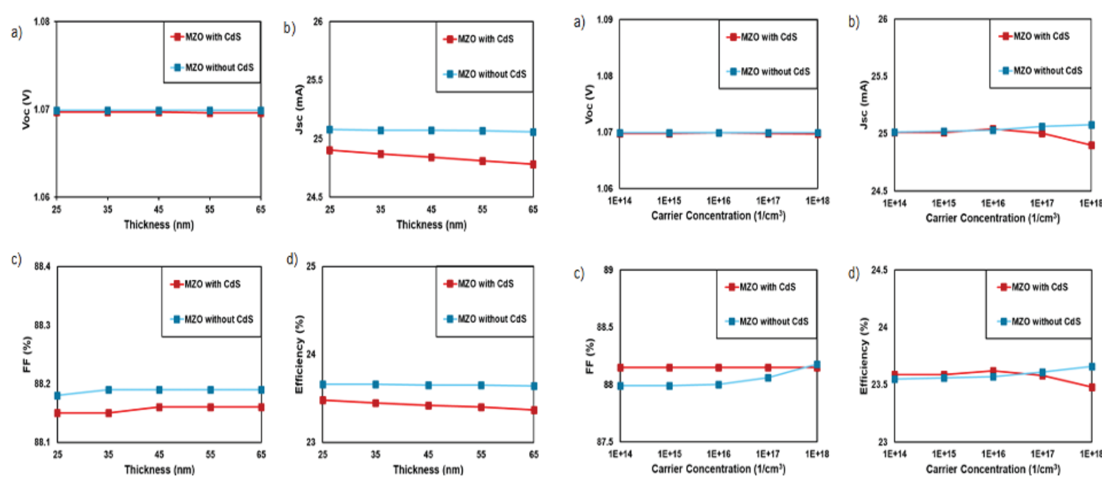

FIGURE 6. Outcome of MZO layer thickness and carrier concentration on solar cell performance

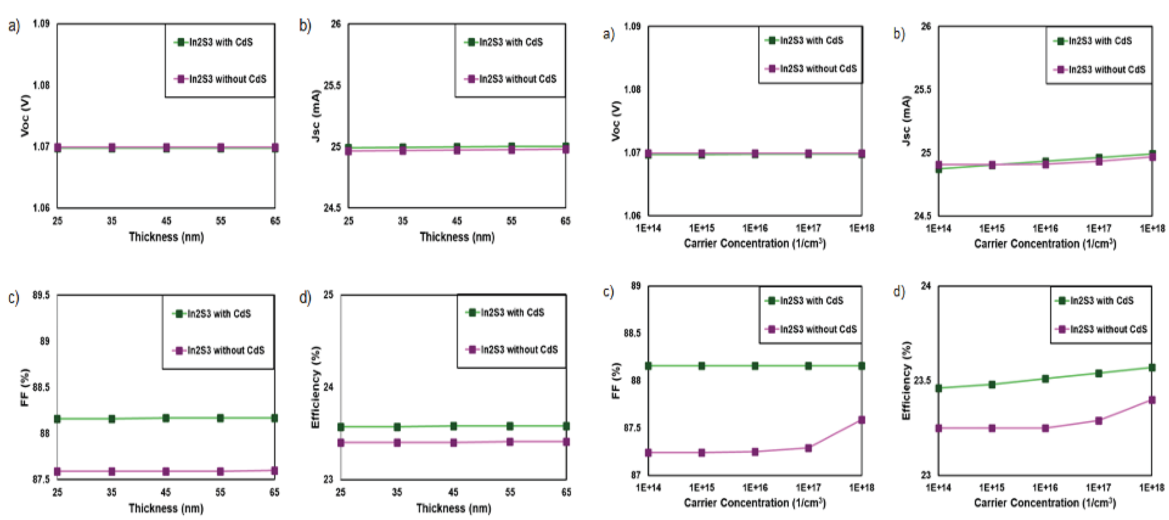

FIGURE 7. Influence of In_2S_3 layer thickness and carrier concentration on solar cell performance

For the Zn_2SO_4 analysis, the V_{OC} and FF of both Zn_2SO_4 structures remain relatively constant with changes in Zn_2SO_4 thickness, as shown in Figure 8, which states the thickness does not affect the recombination or collection of carriers within the device. But as the Zn_2SO_4 layer's thickness increases, the J_{SC} and η increase for both solar cell structures. A thicker Zn_2SO_4 might improve the scattering or absorption of light within the layer, which will lead to a higher number of photogenerated carriers. Thus, for both structures of the Zn_2SO_4 buffer layer, the optimum thickness is 65 nm with obtaining η = 23.66% for Zn_2SO_4 with CdS and η = 22.59% for Zn_2SO_4 without CdS. Structure for Zn_2SO_4 with CdS shows a decrease in J_{SC} and η as the carrier concentration increases due to a high carrier concentration in Zn_2SO_4, which might introduce recombination centers within the layer, hindering the efficient collection of photogenerated carriers. For Zn_2SO_4 without CdS structure, the J_{SC}, FF and η increase with increasing carrier concentration. This suggests that a higher carrier concentration in Zn_2SO_4 improves conductivity. Due to improved conductivity in the Zn_2SO_4 layer, it is reducing carrier recombination. Overall, the results in Figure 8, we can conclude the optimum carrier concentration for Zn_2SO_4 with CdS is 10^{14} cm^{-3} with η = 23.71% and for Zn_2SO_4 without CdS is 10^{18} cm^{-3} with η = 22.59%.

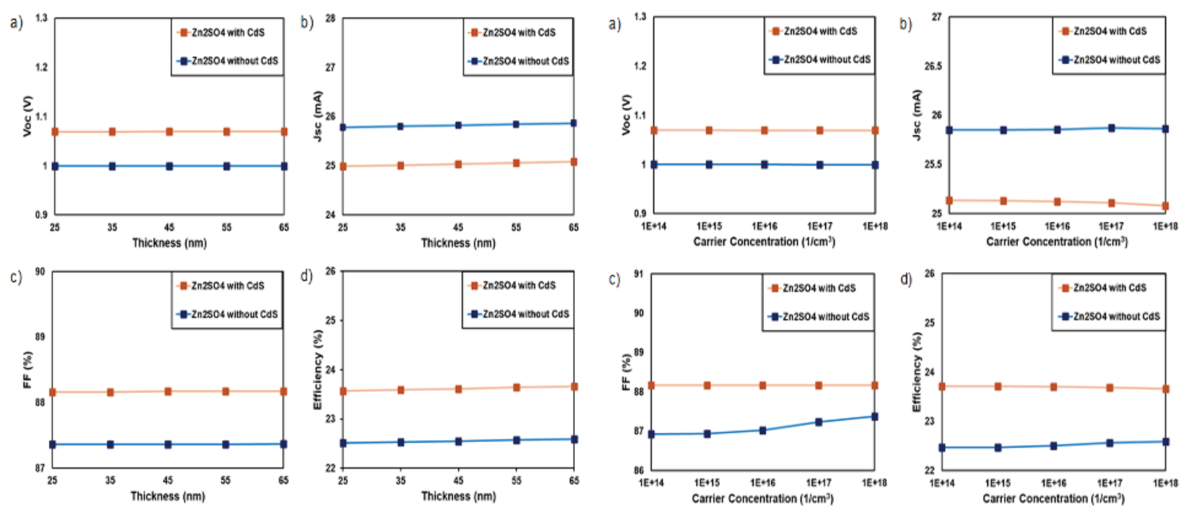

FIGURE 8. Effect of Zn_2SO_4 layer thickness and carrier concentration on solar cell performance

DEFECT ANALYSIS

This study involved introducing defects into all the proposed structures of solar cells in the previous study to analyze the influence of the defect on the performance of the solar cell. We introduce the interfacial defect, which is the defect between the layers, and then vary the defect density. Once done, we will review the effect of defect density on the CdTe solar cell performance with all the baseline and buffer layer structures.

The performance of CdTe solar cells with MZO, In_2S_3, Zn_2SO_4, and baseline structures is depicted in Figure 9 as the defect density rises. The values of the V_{OC} are much less affected by the changes in the defect densities for all structures; therefore, the recombination losses do not seem to affect the solar cell voltage. However, the overall power generation or the short-circuit current density (J_{SC}) slightly reduces for all the structures as the density of defects rises, and it is most affected for the baseline structure. This is because defects in the material are responsible for acting as recombination centers and, therefore, will trap charge carriers, resulting in a low current. Similar to previous results, it is shown that In_2S_3 augments this phenomenon better than the baseline, but MZO and Zn_2SO_4 effectiveness is comparatively better compared to In_2S_3 and the baseline. It is also observed that there is a decrease in the fill factor (FF) with an increase in the defect density, particularly for the baseline structure. Higher defect density can lead to an increase in the series resistance and a corresponding decrease in the shunt resistance, thus giving a lower FF. MZO and Zn_2SO_4 buffer layers ensure a higher FF is attained because interface quality and recombination losses improve.

Therefore, efficiency decreases with an increase in defect density, with the baseline structure most affected. Thus, considering that V_{OC}, J_{SC}, and FF have been reduced, efficiency as the product of these three values is also affected. In other words, the MZO buffer layer has the superior performance among the investigated buffer layers. One can further affirm that it achieves relatively higher J_{SC}, FF, and efficiency even for higher defect density, thus constituting high efficiency in dealing with defect-related. MZO probably refines the interface quality, minimizes the recombination losses and optimizes carrier transport compared to other buffer layers, which ultimately leads to enhanced performance of solar cells under a high density of defects.

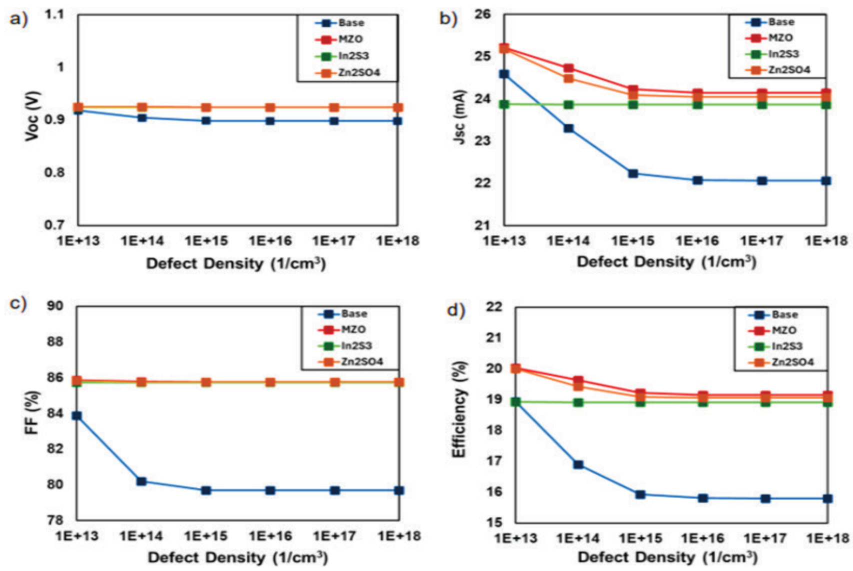

FIGURE 9. Effect of defect density variation

Figure 10 (a) shows J-V characteristics of CdTe solar cells with different structures. Comparing the results of the baseline CdTe structure and the solar cells with buffer layers demonstrates higher current density across the voltage range due to enhanced light absorption and electron-hole pair generation. Both solar cells also reveal slightly enhanced voltage output, which points to the fact that the photogenerated electrons and holes are efficiently separated. Surprisingly, the papers presented results of structures without the CdS layer, and they demonstrated higher performance compared to the structures containing them because of the properties of the buffer layer. The elimination of the CdS layer leads to an optimization of the light absorption and the charge carriers' transport, which, in turn, increases the delivered current and the voltage. Therefore, the structure without the CdS layer is better used as the buffer layer, as seen from the J-V characteristics in Figure 10 (a).

Figure 10 (b) shows the QE of various structures of the CdTe solar cells in function of the wavelength of light. The baseline CdTe structure has significantly lower QE at short wavelengths and, therefore, exhibits the tendency to absorb and convert the incident photons into charges qualitatively worse. Instead, structures that incorporate the buffer layers can show higher QE in short wavelengths because of better absorption characteristics. Most importantly, the structures with buffer layers without CdS perform better than those with the layers of CdS. It can be stated that the presence of the CdS layer deteriorates the optical characteristics at short wavelengths. In general, the creation of extra buffer layers contributes to increasing QE in the short wavelength region, consequently increasing absorption and decreasing reflectance in the solar cell.

TEMPERATURE ANALYSIS

Figure 11 displays the efficiency of CdTe solar cells with MZO, In_2S_3, Zn_2SO_4 and basic structure as the function of working temperature. For all the structures, V_{OC} reduces with the increase in temperature from 300K to 400K because of the enhanced thermal generation of electrons and holes that eventually lead to their recombination. The value of the short-circuit current density (J_{SC}) does not deteriorate under augmentation of the temperature, implying that the photogeneration of the carriers is not influenced much by temperature. On the other hand, fill factor (FF) and efficiency (η) decrease with temperature for all the structures. This is due to the recombination and series resistance increases with the temperatures. Among the buffer layers, the MZO buffer layer displayed high V_{OC}, FF, and η and was comparatively better than In_2S_3, Zn_2SO_4 and the structure without a buffer layer. This indicates that MZO has a better capability of reducing the negative impacts of temperature, possibly because of improved thermal conductivity and fewer recombination losses. Hence, it can be advised that the MZO buffer layer improves the efficiency of solar cells at higher temperatures and can be utilized to increase the thermal performance of CdTe solar cells.

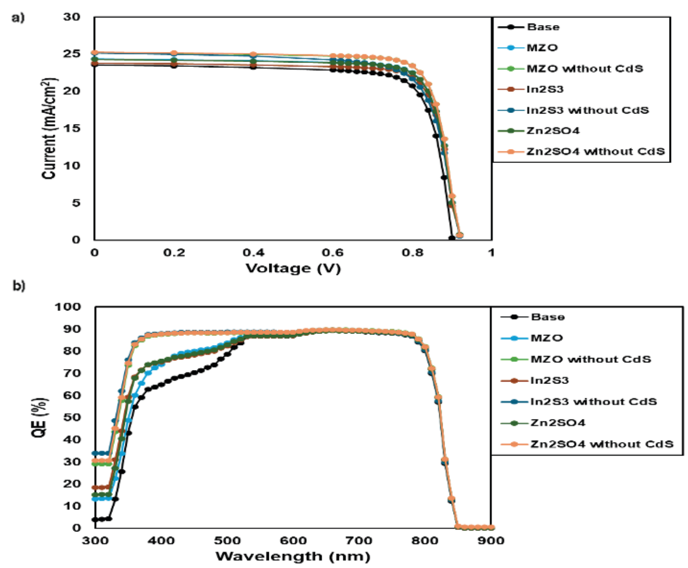

FIGURE 10. (a) J-V and (b) QE measurement for solar cell structures

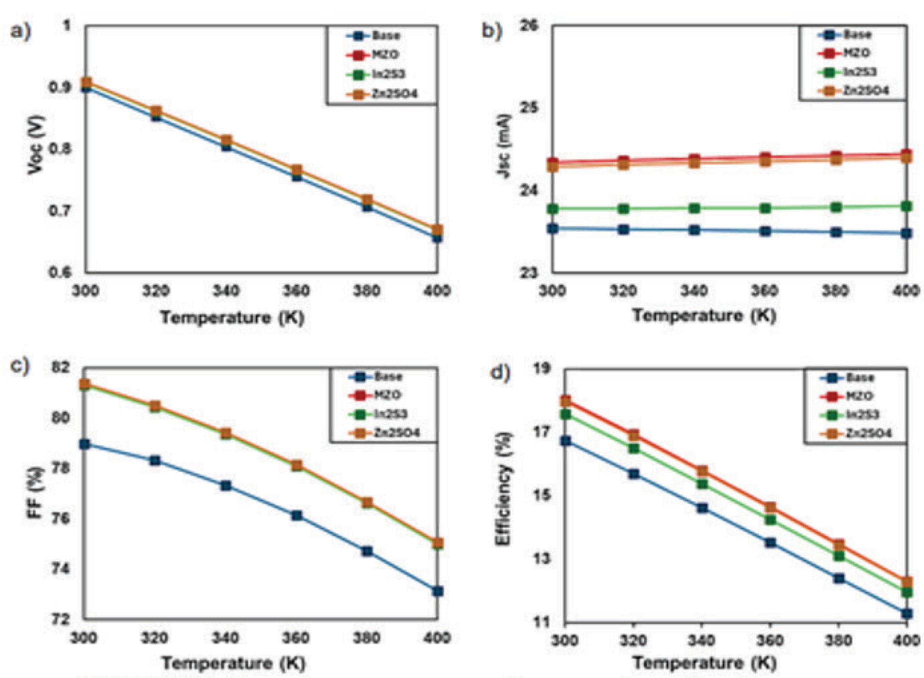

FIGURE 11. Operating temperature effect on solar cell performance

CONCLUSION

The first phase of this study involved the optimization of the base structure to make the maximum efficiency of 22.45%. The second phase assessed the performance according to modification where Magnesium Zinc Oxide (MZO), Indium Sulfide (In_2S_3), and Zinc Sulfate (Zn_2SO_4) buffer layers were introduced, and the structure was changed with the removal of the CdS layer. The solar cell comprising MZO buffer layer without CdS is the most efficient, having an efficiency of 23.66% with the structure

SnO_2/MZO/CdTe, increasing the efficiency of the CdTe solar cell by 1.21%. The optimum MZO carrier concentration is 10^{18} cm^{-3} for MZO without CdS structure. In the third phase, when the defect analysis was conducted and the MZO buffer layer without CdS layer gave a higher efficiency of 18.74%, under the defective conditions compared to the baseline of 16.73%. MZO also showed promising results in the context of interfacial defect evaluation. The final stage examined temperature influences, and it was observed that both MZO and Zn_2SO_4 buffer layers as well as the structure without CdS, had better characteristics at higher temperatures. All in all, the MZO buffer layer without CdS exhibited the highest enhancements in the efficiency of the CdTe solar cell out of all the selected layers.

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DECLARATION OF COMPETING INTEREST

None.

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