Detailed performance analysis of FTO/TiO_2/$FAPbI_3$/CZTS solar cells: Computational study

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ABSTRACT

This study analyzed the performance of FTO/TiO_2/$FAPbI_3$/CZTS solar cells using SCAPS-1D simulations. Various parameters, including thickness, acceptor density, and defect density for the $FAPbI_3$ and CZTS absorber layers, series resistance, shunt resistance, and operating temperature were optimized to enhance device efficiency. The structure consisted of a FTO front contact, TiO_2 as the electron transport layer (ETL), $FAPbI_3$ as the perovskite absorber layer, and CZTS as the secondary absorber layer. The optimized parameters for achieving the highest efficiency included an $FAPbI_3$ thickness of 0.8 µm, a CZTS thickness of 2 µm, and an acceptor density of 10^{16} cm^{-3} for $FAPbI_3$ and 10^{18} cm^{-3} for CZTS. A defect density of 10^{14} cm^{-3} for both absorber layers and an operating temperature of 300 K. Increasing series resistance leads to a decrease in fill factor and efficiency. In contrast, higher shunt resistance enhances the fill factor and efficiency. Under these conditions, the solar cell achieved an open-circuit voltage (V_{OC}) of 1.1148 V, a short-circuit current density (J_{SC}), an overall efficiency (Eta) of 26.17%, and a fill factor (FF) of 87%. These findings contribute significantly to optimizing perovskite/CZTS-based solar cells for improved performance.

Keywords: $FAPbI_3$/CZTS, solar cells, efficiency optimization, heterojunction

1. INTRODUCTION

Perovskite solar cells (PSCs) have achieved impressive advancements, with efficiencies exceeding 25% in recent years [1, 2]. Despite these successes, enhancing their stability and performance remains a critical challenge. Incorporating Copper Zinc Tin Sulfide (CZTS) as an additional absorber layer in a heterojunction solar cell configuration presents a promising solution [3]. This study analyzes the effect of various factors on the performance of formamidinum lead iodide solar cell ($FAPbI_3$) with a CZTS layer. We use SCAPS-1D simulations to examine the impact of absorber layers thickness, acceptor density, defect density, and both series and shunt resistances. Additionally, we investigate how operating temperature influences photovoltaic parameters. By analyzing these aspects, our research aims to provide insights into optimizing PSC performance and stability in this advanced configuration.

2. DEVICE STRUCTURE AND SIMULATION SETUP

The solar cell investigated in this study features a heterojunction structure composed of Glass/FTO/TiO_2/$FAPbI_3$/CZTS/Back contact, as illustrated in Fig.1. The transparent conducting front electrode is fluorine-doped tin oxide (FTO), while TiO_2 serves as the electron transport layer (ETL), efficiently facilitating electron transport and blocking holes [4]. The primary absorber layer is formamidinium lead iodide ($FAPbI_3$), known for its excellent light absorption and charge generation properties [5, 6]. Copper zinc tin sulfide (CZTS) is a secondary absorber layer, enhancing charge separation and collection. The back contact is a metallic layer; in this study, gold (Au) was used as the back contact for its high conductivity and reliability [7-9]. The performance of the designed solar cell was optimized using the Solar Cell Capacitance Simulator (SCAPS-1D), a widely used tool for simulating photovoltaic devices. SCAPS allows detailed control over material properties and device structure, enabling researchers to study the impact of various parameters on solar cell performance [10, 11]. In the simulation, several parameters were varied to optimize the performance of the designed solar cell.

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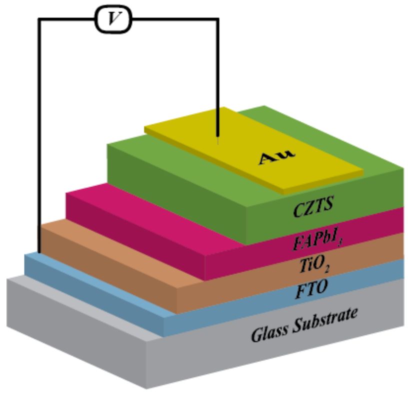

Figure 1. Schematic diagram of the FTO/TiO_2/$FAPbI_3$/CZTS solar cell structure.

The thickness of the $FAPbI_3$ layer was adjusted between 0.2 µm and 0.8 µm, while the CZTS thickness ranged from 0.2 µm to 2 µm. The acceptor density (N_A) for CZTS from 10^{12} to 10^{18} cm^{-3}, and from 10^{12} to 10^{16} cm^{-3} for $FAPbI_3$. The defect density (N_t) was set between 10^{12} and 10^{16} cm^{-3} to examine the effects of recombination on device performance. Additionally, the series resistance (Rs) was varied between 0 Ω.cm^2 and 20 Ω.cm², and the shunt resistance (Rsh) ranged from 200 Ω·cm² to 1800 Ω.cm² to assess their impacts on J-V parameters. Finally, the device was simulated across a temperature range of 300 K to 450 K to investigate the influence of temperature on overall performance. Furthermore, the physical parameters used in the SCAPS simulations are detailed in Table 1 [12, 13].

Table 1. Material parameters for each layer in the solar cell structure.

Parameters	FTO	TiO_2	$FAPbI_3$	CZTS
Thickness(µm)	0.02	0.02	0.8	2
E_g (eV)	3.5	3.26	1.5	1.45
χ (eV)	4	4.2	4	4.5
ε_r (eV)	9	9	6.6	10
N_C (cm^{-3})	2.2×10^{18}	2.2×10^{18}	1.2×10^{19}	2.2×10^{18}
N_V (cm^{-3})	2.2×10^{18}	1.8×10^{18}	2.9×10^{18}	1.8×10^{19}
μ_e (cm^2/ V.s)	20	20	2.7	100
μ_h (cm^2/ V.s)	10	10	1.8	25

3. RESULTS AND DISCUSSION

The SCAPS simulations for the FTO/TiO_2/$FAPbI_3$/CZTS solar cell structure reveal significant insights into how various parameters affect device performance. Fig.2 illustrate the results of varying the CZTS thickness from 0.2 µm to 2 µm at different fixed $FAPbI_3$ thickness values (0.2 µm, 0.4 µm, 0.6 µm, and 0.8 µm). At an $FAPbI_3$ thickness of 0.2 µm, increasing the CZTS thickness improves V_{OC} from 1.0024 V to 1.04 V, JSC from 20.94477 mA/cm^2 to 21.10932 mA/cm^2, and efficiency from 17.47 % to 18.62 %. At an FAPbI3 thickness of 0.4 µm, similar trends are observed: V_{OC} rises from 1.0154 V to 1.0443 V, J_{SC} from 25.9713 mA/cm² to 27.7176 mA/cm^2, and efficiency from 21.80% to 24.14%. These improvements continue as $FAPbI_3$ thickness increases, with V_{OC} reaching 1.1148 V, JSC reaching 28.3979 mA/cm^2, and efficiency peaking at 27.19 % for a CZTS thickness of 2 µm when the $FAPbI_3$ thickness is set at 0.8 µm. These results indicate that optimizing both CZTS and $FAPbI_3$ thicknesses enhances the light absorption and charge collection efficiency of the solar cell, leading to improved overall performance.

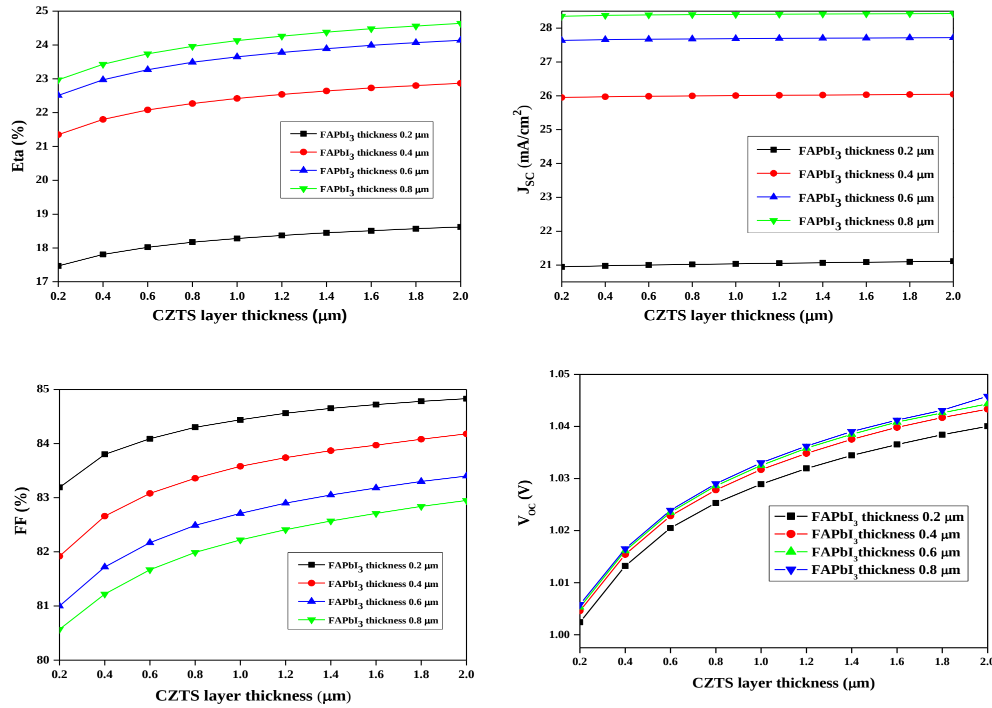

Figure 2. Effect of $FAPbI_3$ and CZTS layer thickness on solar cell performance parameters.

Examining the effect of varying acceptor density in both CZTS and $FAPbI_3$, When the $FAPbI_3$ acceptor density is set to 10^{10}, 10^{12}, 10^{14}, and $10^{16} cm^{-3}$, increasing the CZTS density from $10^{12}$to 10^{18} cm^{-3} raises V_{OC} from 0.7956 V to 1.1141 V and efficiency from 16.59 % to 27.19%. When varying the acceptor density in $FAPbI_3$, similar improvements are observed in both J_{SC} and FF. The optimal performance occurs at an acceptor density of $10^{18} cm^{-3}$ for CZTS and $10^{16} cm^{-3}$ for $FAPbI_3$, indicating enhanced charge transport and reduced recombination losses with higher acceptor densities (see Fig.3).

The SCAPS simulations also explore the effect of defect density in both CZTS and $FAPbI_3$ on device performance. Reducing the defect density in CZTS from $10^{16} cm^{-3}$ to $10^{12} cm^{-3}$while keeping the defect density in $FAPbI_3$ constant at $10^{10} cm^{-3}$ improves V_{OC} from 1.0786 V to 1.0851 V and efficiency from 26.03 % to 26.39 %. When varying the defect density of CZTS from $10^{16} cm^{-3}$ to $10^{12} cm^{-3}$ with the $FAPbI_3$ defect density set at $10^{14} cm^{-3}$, the V_{OC} increases from 1.0936 V to 1.0966 V and efficiency from 25.88 % to 27.19 %. Lastly, with the $FAPbI_3$ defect density set at $10^{16} cm^{-3}$, a reduction in the CZTS defect density similarly boosts performance, with V_{OC} rising from 0.9274 V to 0.9277 V and efficiency from 17.11% to 17.27 %. These improvements highlight the importance of minimizing defect densities to reduce recombination losses and enhance overall device performance (see Fig.4).

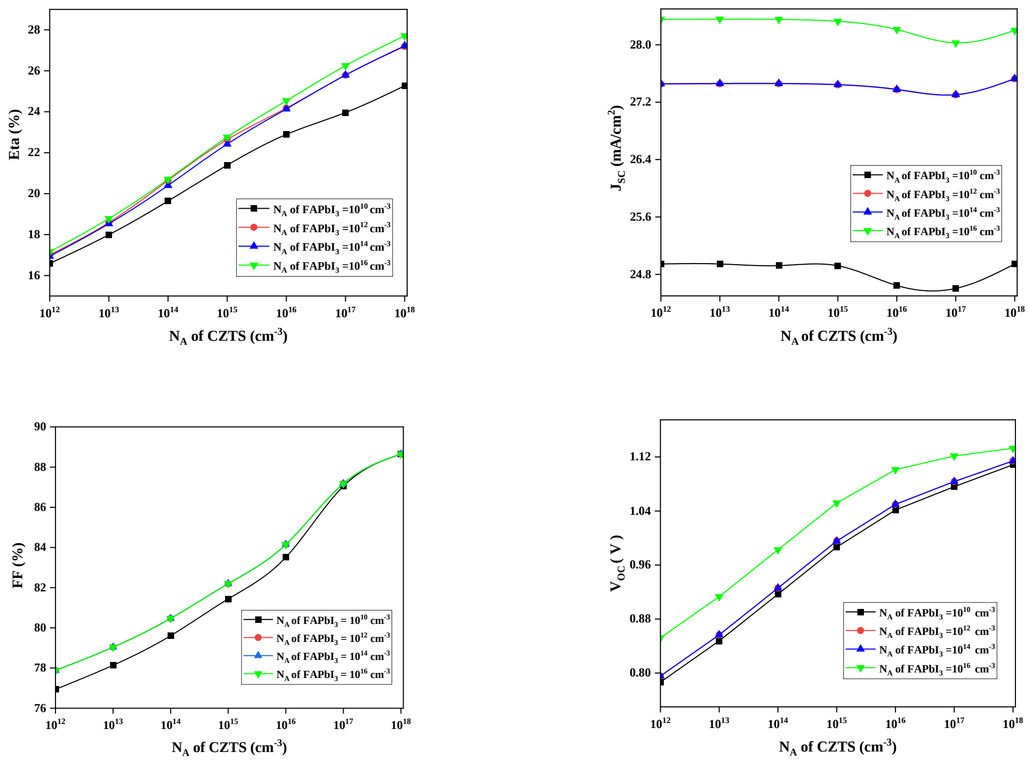

Figure 3. Impact of acceptor densities in $FAPbI_3$ and CZTS on photovoltaic parameters.

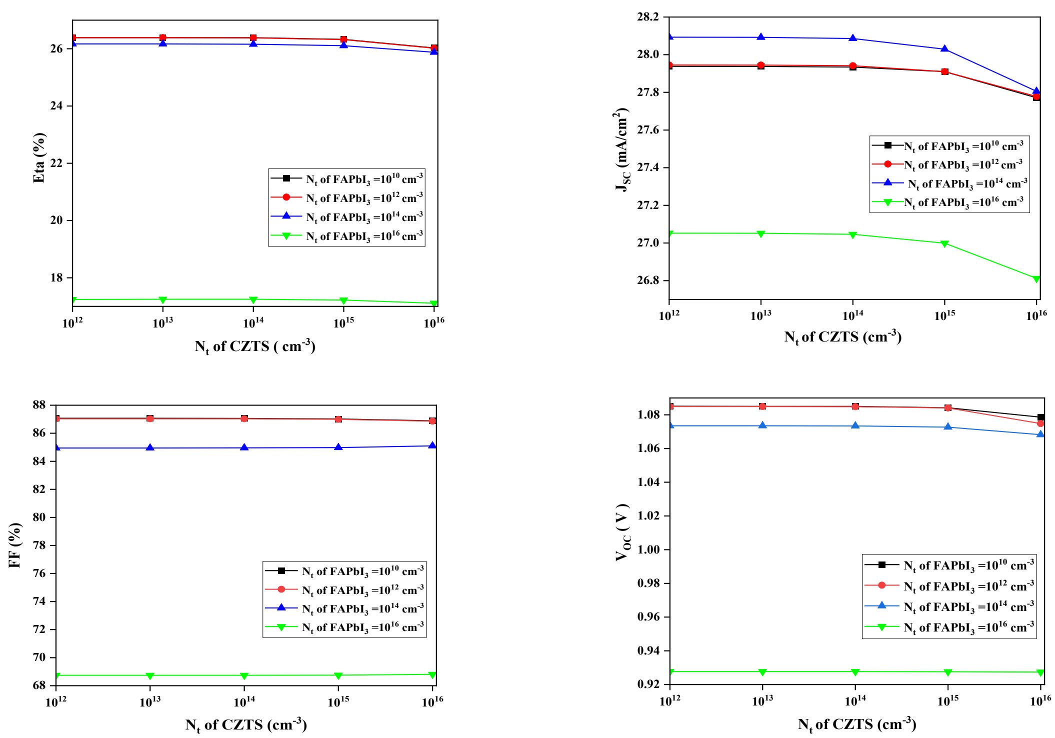

Figure 4. Impact of defect densities in $FAPbI_3$ and CZTS on photovoltaic parameters.

The effects of series and shunt resistance on the solar cell were significant. Increasing series resistance from 0 Ω to 20 Ω resulted in efficiency decreasing from 27.37% to 20.68%. Additionally, reducing shunt resistance from 1800 Ω to 200 Ω caused efficiency to drop from 26.94% to 16.63% as shown in Fig.5. These results underscore the importance of minimizing series and shunt resistances to maintain high efficiency.

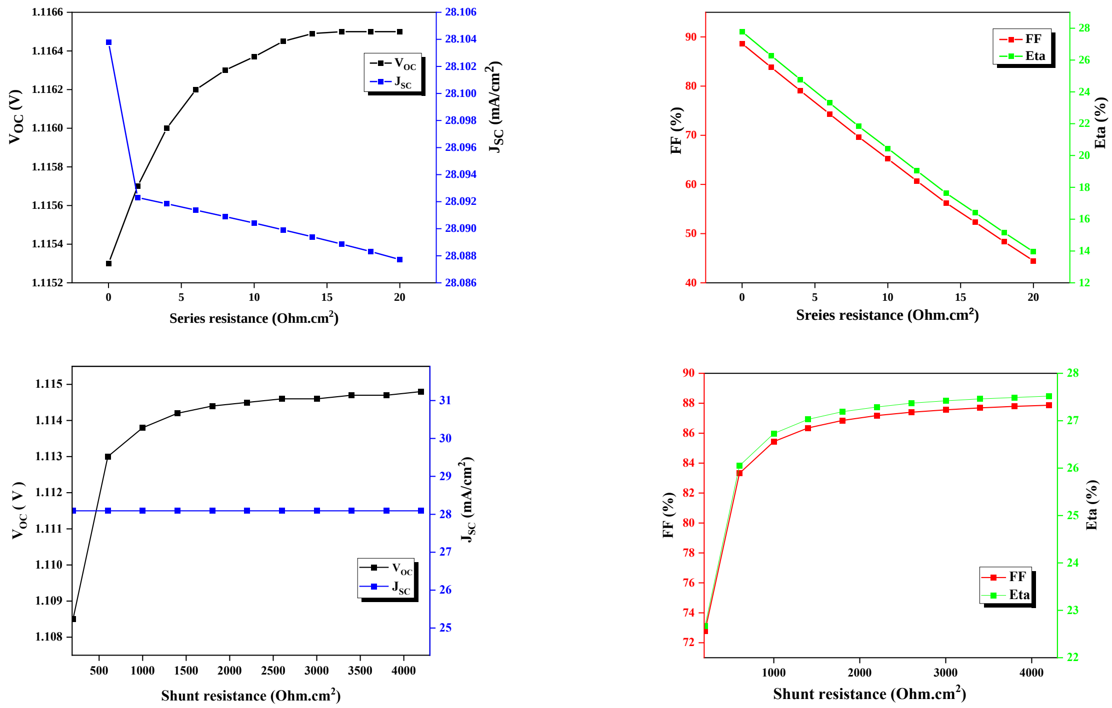

Figure 5. Impact of series and shunt resistance on V_{OC}, J_{SC}, FF, and efficiency of the solar cell.

Finally, the influence of temperature on performance was analyzed as shown in Fig.6. Increasing the temperature from 300 K to 450 K led to a decrease in V_{OC} from 1.1486 V to 0.9705 V and a reduction in efficiency from 27.37% to 21.95%. This temperature dependency highlights the adverse effects of elevated operating temperatures on device performance, likely due to increased recombination and reduced semiconductor band gap.

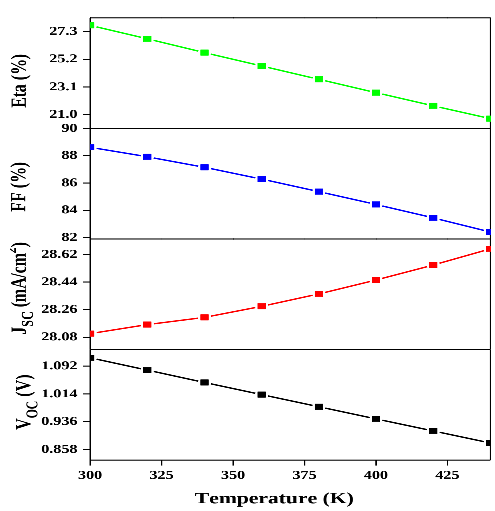

Figure 6. Impact of temperature variations on solar cell performance.

4. CONCLUSION

The SCAPS-1D simulations of the FTO/TiO_2/$FAPbI_3$/CZTS solar cell structure have provided valuable insights into optimizing device performance through various parameters. The study identified that increasing CZTS thickness improves performance metrics, with the highest efficiency of 27.19% achieved with a CZTS thickness of 2 µm and a $FAPbI_3$ thickness of 0.8 µm. Similarly, optimizing acceptor densities for both CZTS and $FAPbI_3$ significantly enhances performance, with peak efficiency reached at 10^{18} cm^{-3} for CZTS and 10^{16} cm^{-3} for $FAPbI_3$. Reducing defect densities in both absorber layers leads to higher V_{OC} and efficiency, emphasizing the importance of minimizing defects to reduce recombination losses. The study also highlighted that lower series resistance and higher shunt resistance are crucial for maintaining high efficiency, while increased temperature adversely affects device performance by reducing V_{OC} and efficiency. Overall, the findings underscore the importance of carefully optimizing absorber layer thickness, acceptor density, defect density, series and shunt resistances, and operating temperature to maximize the efficiency and performance of the FTO/TiO_2/$FAPbI_3$/CZTS solar cell structure. Future research should further refine these parameters and exploring additional strategies to enhance solar cell performance.

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