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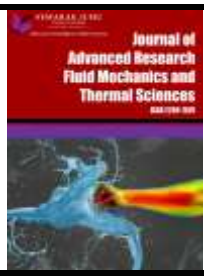

Optimizing CZTS Solar Cells Efficiency using Eco-Friendly Layers by SCAPS Simulation

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ABSTRACT

This study delves into the simulation of CZTS (Copper Zinc Tin Sulfide) solar cells, with a primary focus on the incorporation of environmentally sustainable layers. By conducting extensive simulations, we systematically analyze the performance of CZTS solar cells, emphasizing the utilization of eco-friendly materials. Our research encompasses a range of aspects, such as employing the SCAPS-1D software to simulate the foundational MoS_2/CZTS/TiO_2/ITO:Al structure in order to assess the optimal efficiency of three different CZTS-based solar cells enhanced with MoS_2. This involved modifying the thickness of the absorptive layer in each cell and fine-tuning the thickness of MoS_2. Moreover, we observed the temperature-dependent behavior of CZTS cells, which is linked to the rise in electron energy levels with increasing temperatures, consequently affecting the bandgap. In order to boost the performance of solar cells, we carried out a detailed analysis of the work function of the rear contact. Our computational evaluations decisively propose platinum as a more beneficial option than molybdenum for the back metal contact. Additionally, our results indicated that platinum could serve as a favorable back contact choice with an efficiency of 20.9151%.

1. Introduction

Given the continuing growth in global energy demands, researchers are increasingly exploring sustainable and renewable alternatives to current production methods. This has led to a heightened focus on developing innovative strategies to meet these needs. Among the various sustainable options, solar energy stands out as an inexhaustible source with significant potential for clean power generation, is a significant source of renewable energy. Photovoltaic cells, also known as solar panels, are capable of converting solar energy into electrical energy, making solar energy an attractive

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option. Nowadays, the technology of solar cells, a significant accent has been put on the production of semiconductor absorber layers with thin layers, in particular those based on the Chalcopyrite (CIGS) [1-5]. This is mainly due to their exceptional efficiency, exceeding 20%, which surpasses most of the alternatives currently available [6]. Cdte, another thin layer of absorbent, is also remarkable for its effectiveness. However, the broad acceptance of CIGS and CDTE in solar cell technology has faced significant obstacles marked by formidable challenges. These challenges encompass not only the prohibitive costs associated with their implementation but also extend to the diminishing availability of indium (In) and heightened concerns surrounding the toxicity attributed to cadmium (Cd).

The progression of photovoltaic cell technology has led to the creation of solar panels engineered to optimize the utilization of sunlight. These cells incorporate a diverse array of materials, such as silicon, rare earths, and plastics, each possessing distinct advantages and drawbacks. Within this diverse landscape, the potential of solar devices to provide long-lasting, cost-efficient, and eco-friendly energy is emphasized through the use of organic-polymer materials known for their adaptability and scalability. Nonetheless, challenges like exposure to air, humidity, ultraviolet radiation, water, and heat pose risks to the efficiency and longevity of these devices. In response to these challenges, thin-film solar cells are being increasingly recognized as a viable solution. The commonly utilized absorptive layer, chalcopyrite Cu semiconductor (In, Ga)Se_2 (CIGS), has exhibited efficacy, yet its dependence on scarce and hazardous elements like In and Cd presents notable drawbacks. To overcome these limitations, researchers are shifting towards the utilization of the cost-effective Cu2ZnSn (S, Se)4 (CZTS) adsorption layer.

CZTS, being a semiconductor, exhibits notable photovoltaic characteristics due to its direct band gap, high absorption coefficient, and optimal band energy ranging from 1 to 1.5 electron volts (eV). These intrinsic properties establish CZTS as a promising candidate for solar photovoltaic purposes, facilitating the effective conversion of solar energy into electricity. Moreover, CZTS is abundant, eco-friendly, and economically viable, sourced from metals devoid of rare-earth elements. This abundance and environmental friendliness render CZTS an appealing substitute for conventional materials, thereby fostering the progression of sustainable solar energy technologies [1-5].

Additionally, CZTS technology addresses the limitations posed by scarce and hazardous components found in conventional solar cells. By utilizing CZTS, which consists of elements abundant in the Earth's crust and non-toxic in nature, the solar industry can overcome environmental and health challenges associated with materials such as cadmium and tellurium. The shift towards CZTS represents a significant progress towards environmentally conscious and sustainable energy solutions, ensuring efficient energy generation while prioritizing environmental protection.

In this study, an approach that the completion does not take into account the properties of materials has been adopted for digital simulation, focusing on the implementation of a thin layer of absable. Using data -based information, the initial configuration of the device has been meticulously formulated to establish a robust base for all simulations. The selection of an appropriate material for the slim absorption layer has been determined by an evaluation of the configuration of the experimental device field, which served as a reference for the simulation process for its exceptional and distinctive properties [6,7].

2. Methodology

2.1 Simulation

Numerical analysis has become a crucial tool in the development of various devices, including thin-film solar cells (TFSCs). Leveraging simulation tools such as SCAPS 1D, researchers can enhance

the precision of predicting the performance and energy efficiency of these devices across diverse conditions.

The software SCAPS 1D version 3.307 was developed by the Department of Electronics and Information Systems (ELIS) at the University of Gent in 2012, specifically designed for simulating the field layer and blaze diffractive grating of Thin-Film Solar Cells (TFSCs). Drawing on a foundation of literature and experimental results, the software incorporates various parameters, each meticulously referenced. Among the pivotal parameters employed within SCAPS, the pre-factor Aα holds significance. It is set at 105 to calibrate the absorption coefficient calculated through a specific equation. This numerical value is grounded in research studies such as those conducted by Burgelman *et al.,* [10], Kotipalli *et al.,* [8], and Kannaujiya *et al.,* [9].

$$\alpha = A_{\propto}(hv - E_g)^{\frac{1}{2}} \tag{1}$$

The simulation is conducted under conditions of 1 Sun illumination, with an incident power density of 1000 W/m^2 and a temperature of 300 K. This involves applying well-established equations, including the continuity equation, Poisson's equation, and the electron/hole transport equation, accounting for various recombination mechanisms. These computations are aimed at capturing and replicating the behavior of Thin-Film Solar Cells (TFSCs). Conducting these simulations holds significant importance in the refinement of both the design and performance aspects of Thin-Film Solar Cells (TFSCs), striving for optimal efficiency and cost-effectiveness. As the global demand for renewable energy solutions continues to rise, the utilization of numerical analysis software such as SCAPS 1D is poised to gain even greater prominence in the ongoing development of sustainable energy sources [10].

$$\frac{\partial \mathrm{n}}{\partial t} = \frac{1}{q} div\overrightarrow{J_n} + G_n - R_n \tag{2}$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} div\overrightarrow{J_p} + G_p - R_p \tag{3}$$

In the simulation of thin film solar devices, careful consideration of the overall discontinuity parameter is crucial. However, in a recent study, this vital parameter was overlooked, and instead, electrical and optical parameters were sourced from existing literature while maintaining a temperature of 300 K. The solar cell was subjected to illumination with a Global Spectrum of 1000Wbm-2 and an Air Mass value of 1.5, chosen based on previous studies. Additionally, input material characteristics for each layer of the SCAPS 1-D tool, as well as device parameters, were adjusted as needed. Despite the omission of the overall discontinuity parameter, this simulation approach yielded valuable insights into the behavior of thin film solar devices. It is recommended that future studies consider incorporating the overall discontinuity parameter to enhance the precision of simulations.

2.2 Device Configuration

The foundation of this software relies on equations related to semiconductors, specifically the continuity equation for electrons (4), continuity equation for holes (5), and the Poisson equation [11]

$$\frac{\partial j_n}{\partial x} + G_n - U_n(n,p) = 0 \tag{4}$$

$$\frac{\partial j_p}{\partial x} + G_p - U_p(n,p) = 0 \tag{5}$$

$$\frac{d^2\Psi}{d^2x} = \frac{dE}{dx} = -\frac{\rho}{\varepsilon_r \varepsilon_0}(p - n + N_D^+ - N_A^-) \tag{6}$$

The equations that describe the drift-scattering of electrons and holes during carrier transport are as follows

$$j_n = qn\mu_n E + qD_n \frac{\partial n}{\partial x} \tag{7}$$

$$j_p = qn\mu_p E - qD_p \frac{\partial p}{\partial x} \tag{8}$$

Einstein's equation provides a relationship between the scattering efficiency, carrier mobility, and carrier lifetime

$$D_{(n,p)} = \sqrt{\mu_{(n,p)} \frac{KT}{q} \tau_{(n,p)}} \tag{9}$$

The efficiency (PCE) and the fill factor are showing as

$$FF = \frac{P_{max}}{P_t} = \frac{V_{max} J_{max}}{V_{oc} I_{sc}} \tag{10}$$

$$PCE = \frac{V_{oc} I_{sc}}{P_{in}} FF \tag{11}$$

In our research, we explore the intricate design and simulation of an innovative solar cell configuration with the goal of maximizing energy harvesting efficiency. Central to this undertaking is a meticulous focus on material selection and interface engineering, alongside the utilization of advanced simulation techniques employing SCAPS 1-D software.

The solar cell structure, depicted in Figure 1, is intricately developed to enhance light absorption and the transport of charge carriers. Each layer within this multi-layered device plays a vital role in its overall functionality, with distinct properties contributing to its efficacy. The transparent conductive layer utilizing Indium Tin Oxide (ITO) serves as a window layer, enabling light entry while upholding electrical conductivity. This layer is characterized by its high transmittance in the visible spectrum, ensuring optimal penetration of light into the solar cell. Positioned strategically, the absorber layer composed of Copper Zinc Tin Sulfide (CZTS) effectively captures photons and produces charge carriers. Its chemical composition and crystalline structure are meticulously examined to achieve maximum solar light absorption and conversion efficiency. Titanium Dioxide (TiO_2), functioning as a buffer layer, is distinguished by its electron transport characteristics and ability to reduce recombination losses.

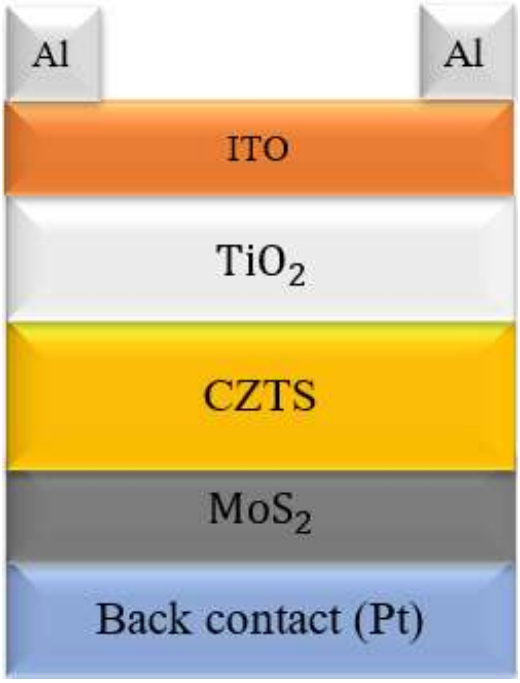

Fig. 1. The structure of the proposed device

The porosity and specific surface area of TiO_2 are critical for facilitating charge carrier transport and minimizing electrical losses in the device. The Platinum (Pt) layer, serving as a back contact, is chosen for its outstanding electrical conductivity and compatibility with CZTS. Its morphology and adhesion to the absorber layer are essential for ensuring the effective extraction of charge carriers generated within the solar cell. The Back Surface Field (BSF) layer, comprised of Molybdenum Disulfide (MoS_2), is a promising semiconductor material due to its appropriate band gap of 1.230 eV and the van der Waals bonding formed by stacked monolayers. Furthermore, MoS_2 possesses unique properties such as its inert character and insensitivity to O_2 and some acids.as SCAPS 1-D automatically calculates the work function to establish ohmic contact. Overall, this solar cell device configuration presents a promising solution for efficient energy harvesting [12,13]. Extensive research is conducted on its charge carrier transport properties to mitigate surface recombination losses and enhance charge carrier collection efficiency in the solar cell.

The optimization of solar cell configuration is greatly dependent on numerical simulation. In order to enhance the efficiency of solar cells, SCAPS numerical simulations are utilized to ascertain the optimal thicknesses of the absorber, buffer, and BSF layers, along with other essential parameters of photovoltaic cells. The performance parameters of the solar cell are provided in Table 1.

In this study, the SCAPS-1D software is employed to examine the attributes of the solar cell, such as thickness, temperature, and characteristics of the front contact, with a specific focus on the CZTS layer subsequent to the addition of a hole transport layer (HTL) between CZTS and the rear contact. MoS_2 is utilized as the HTL, playing a dual function as an intermediary layer. The HTL induces a pushing force towards the rear of the heavily doped device, aiding in the transportation of minority carriers towards the depletion region and therefore passivating the rear surface. In the absence of an HTL, a large portion of carriers remain inadequately utilized at the rear contact; hence, the integration of an HTL like MoS_2 in the suggested solar cell allows for complete carrier utilization. As a result, the HTL channels the majority of carriers towards the absorber layer, resulting in an improved efficiency of the solar cell.

MoS_2, serving as the hole transport layer (HTL), facilitates the collection of holes towards the back contact of the solar cell due to a rapid transition in the valence band. This property helps reduce

recombination phenomena within the solar cell, leading to improvements in electrical characteristics such as fill factor (FF), short-circuit current density (Jsc), and open-circuit voltage (Voc). Moreover, the incorporation of MoS_2 as the HTL enables an enhancement in power conversion efficiency (PCE) even with a reduced thickness of CZTS compared to conventional.

Table 1
The parameters used in this simulation

Parameters	CZTS	MoS_2	TiO_2	ITO
thickness (μm)	Var	0.1	0.125	0.05
dielectric permittivity (relative)	10	3	10	8.9
Electron mobility (cm^2/V.s)	100	100	100	10
hole mobility (cm^2/V.s)	25	150	25	10
shallow uniform donor density ND (cm^{-3})	10	10	10^{17}	10^{20}
shallow uniform acceptor density NA (cm^{-3})	$2 * 10^{17}$	10^{17}	0	0
bandgap (eV)	1.50	1.29	3.2	3.65
Nc (cm^{-3})	$2.2 * 10^{18}$	$2.2 * 10^{18}$	$2.0 * 10^{17}$	$5.2 * 10^{18}$
Nv (cm^{-3})	$1.8 * 10^{19}$	$1.8 * 10^{19}$	$6.0 * 10^{17}$	10^{19}
electron affinity (eV)	4.5	4.2	4.2	4.8
Electron thermal velocity (cm/s)	10^7	10^7	10^7	$2 * 10^{17}$
hole thermal velocity (cm/s)	10^7	10^7	10^7	10^7

3. Results

3.1 Examining the Impact of Absorber Layer Thickness

The thickness of the absorbing layer is of paramount importance, because it essentially determines the main dimension of the solar thin film structure, In the CZTS solar cell, the hole transport layer known as MoS_2, often referred to as back surface field (BSF). We investigated the electrical characteristics of the photovoltaic cell by varying the thickness of the absorber in a range of 400 nm The impact of changing the thickness of the absorbing layer on parameters such as Voc, Jsc, FF and PCE is shown in Figure 2 we observe in the figures Voc, Jsc and PCE all show an increase as the thickness of the CZTS absorbing layer increases, considering MoS_2 as the BSF layer.

This suggests that more photons are absorbed, thus leading to the generation of a greater number of electron-hole pairs [14]. In Figure 2(d), the increase in "Voc" can be attributed to the large bandgap of MoS_2. It is a paper that increases the bandgap, as mentioned by Ghorbani *et al.,* [15], this increase corresponds to Voc. In Figure 2(c), the fill factor (FF) curves of the solar cell initially show a minor increment, followed by a subsequent decrease of 0.6 μm, indicating that MoS_2 remains largely insensitive to thickness changes of the CZTS absorbent layer. This behavior can be attributed to the dominant role of recombination phenomena within the cell. In Figure 2(a), the power conversion efficiency (PCE) of the photovoltaic cell shows a notable increase up to 1.0 μm, indicating a substantial improvement. This improvement is mainly attributed to the reduction in parasite resistance. The higher bandgap of CZTS allows the absorption of a greater number of carriers. This phenomenon aligns well with the Beer-Lambert law $I = I_0 e^{(-\propto x)}$, providing a more precise understanding of the increased surface absorption within the CZTS absorbing layer, leading to

enhanced photogeneration. Therefore, this achievement contributes to the superior performance of the solar cell, as argued by Dwivedi [16].

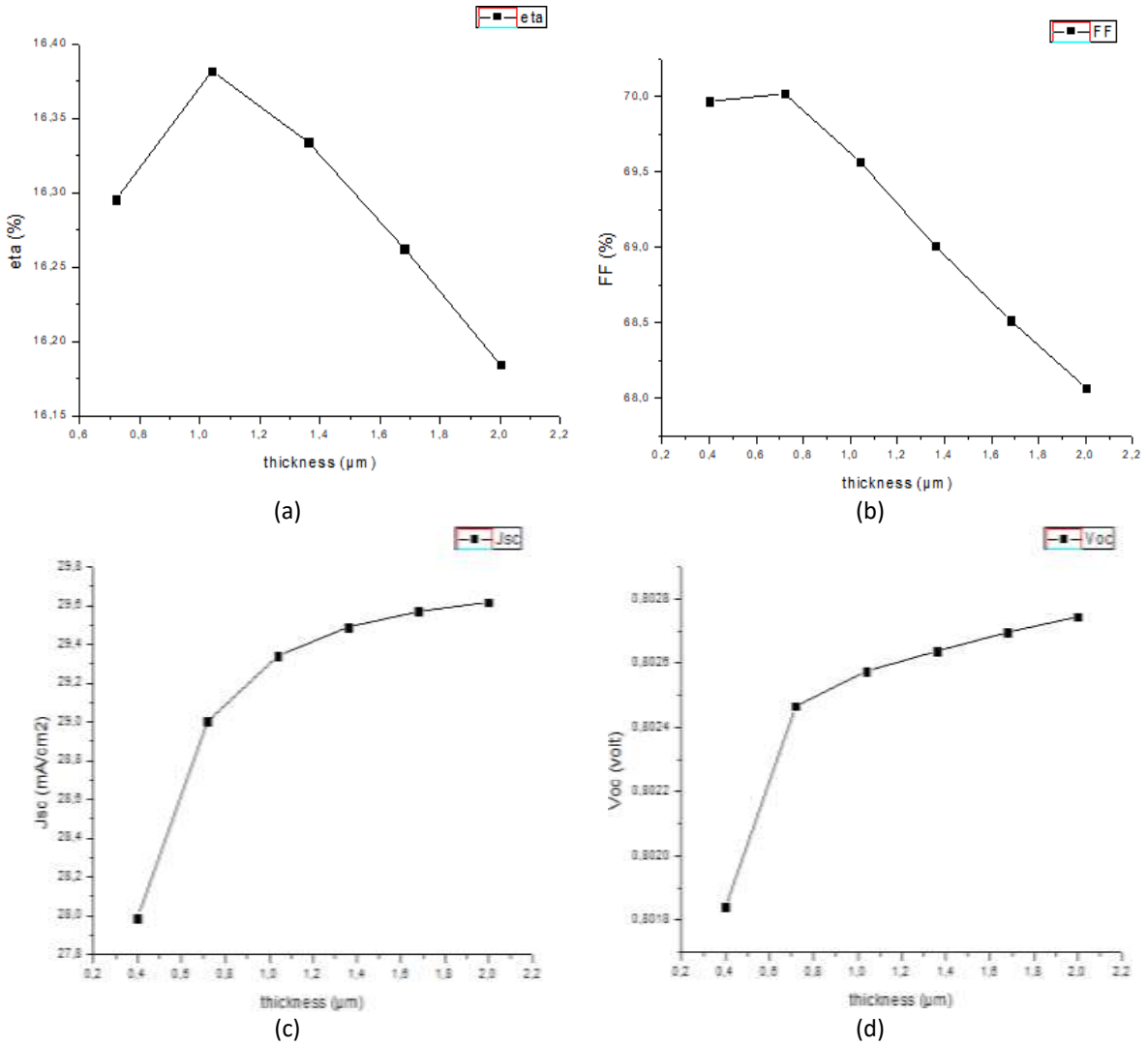

Fig. 2. Variation of cell efficiency, (a) eta, (b) FF, (c) Jsc and (d) Voc with CZTS thickness

3.2 Examining the Impact of Temperature Variation

The temperature undergoes significant variations across many regions of the globe, and solar cells find numerous applications in diverse locations worldwide. Therefore, it is crucial to investigate the output characteristics of photovoltaic cells over a wide temperature range, given the sensitivity of solar cell output performance to thermal fluctuations. Thus, the operational temperature range has been adjusted from 300 K to 400 K, within the conditions of AM 1.5 and the fist level of illumination of sun. The short-circuit current (Jsc) of the cell with MoS_2 shows a slight increase, whereas the Jsc of the cell mentioned by Dwivedi [16] appears to remain constant with the temperature rise. The reason for the decrease in open-circuit voltage (Voc) and the slight increase in Jsc lies in the sensitivity of MoS_2 to temperature changes. At higher temperatures, there is a notable decline in Voc, leading electrons to gain sufficient energy for recombination with holes before reaching the depletion region and being collected [17,18]. The narrowing of the energy bandgap leads to an overproduction of photons, providing the requisite energy to generate a pair of electrons and holes as depicted in Figure 3(a) [19].

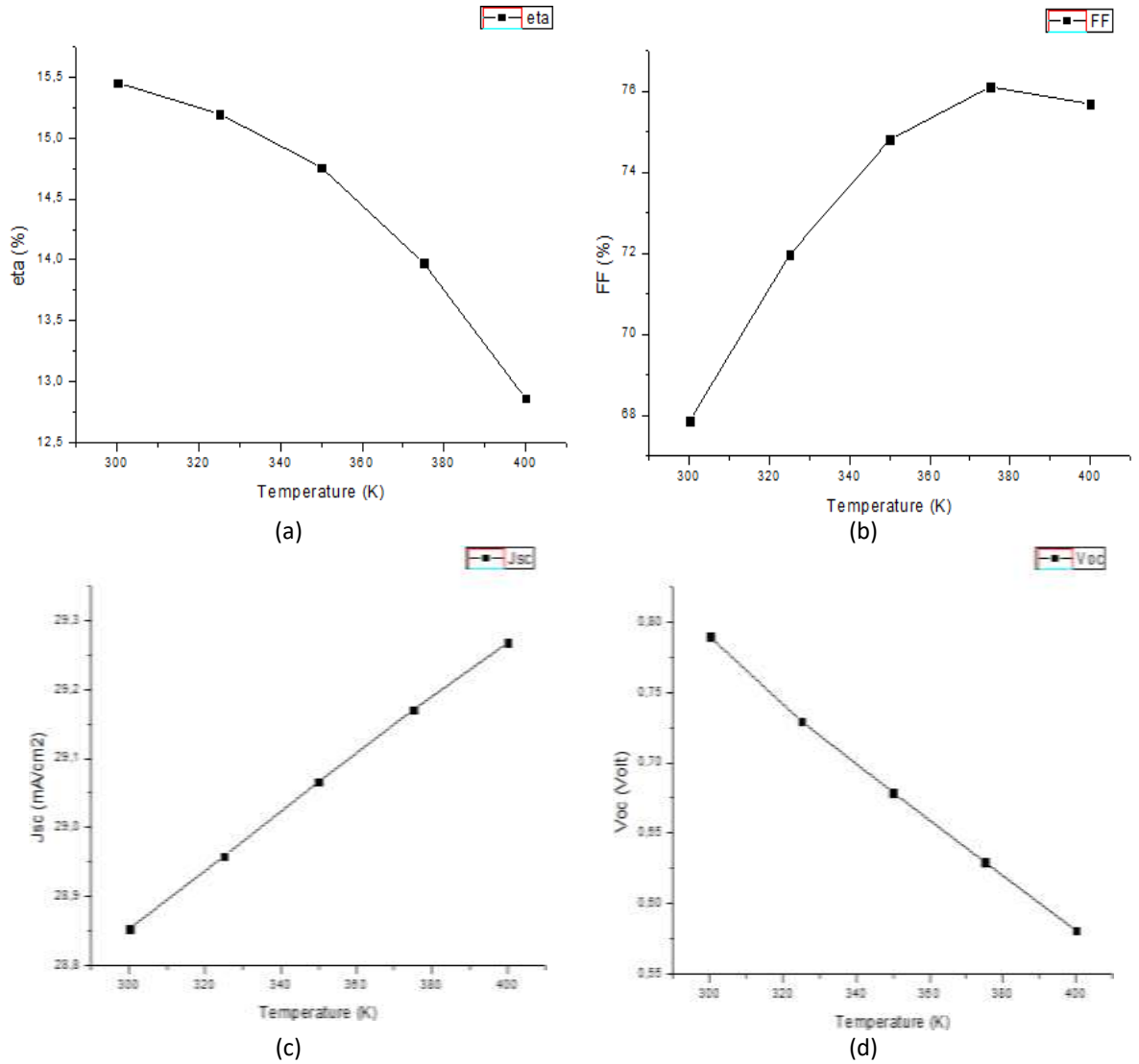

Fig. 3. Variation of cell efficiency, (a) eta, (b) FF, (c) Jsc and (d) Voc with temperature effect

The open-circuit voltage (Voc) is ascertained through the utilization of Eq. (1)

$$V_{oc} = \frac{kT}{q} ln\left(\frac{I_{sc}}{I_0}\right) = \frac{kT}{q}[lnI_{sc} - lnI_0] \quad (1)$$

The relationship between the decrease in Voc and the escalation in Jsc as temperature rises is validated by Eq. (1), which establishes a connection between Voc and the saturation current I_0.

$$V_{oc} = \frac{1}{q}E_g \quad (2)$$

Eq. (2) validates that with the rise in temperature, there is a decrease in Voc which consequently leads to a significant reduction in the bandgap, thereby causing a collective influence on Voc, Jsc, FF, and PCE.

3.3 Examining the Impact of Interfacial Layer

The study focused on the influence of back surface fields (BSF) on the performance of a photovoltaic (PV) cell. By varying the thickness of the MoS_2 back surface fields in the range of 0.2 to

0.3 µm, a continuous increase is observed in the curves of Figure 4(b) and Figure 3(d). Figure 3(a) also reveals an increase in power conversion efficiency (PCE) in the presence of MoS_2. This phenomenon can be attributed to increased reflection of photons by MoS_2 [20]. MoS_2 exhibits special characteristics, including a high Seebeck coefficient and a wide bandgap, explaining the variations observed in the Voc, Jsc, FF and PCE parameters, as shown in the figures. The short circuit current density (Jsc) is slightly higher, mainly due to the ability of MoS_2 to facilitate rapid charge transport. More precisely, here are the results obtained: PCE =16.6684%, FF = 68.5442%, Jsc = 30.11985173 mA/cm^2 and Voc = 0.807367 V.

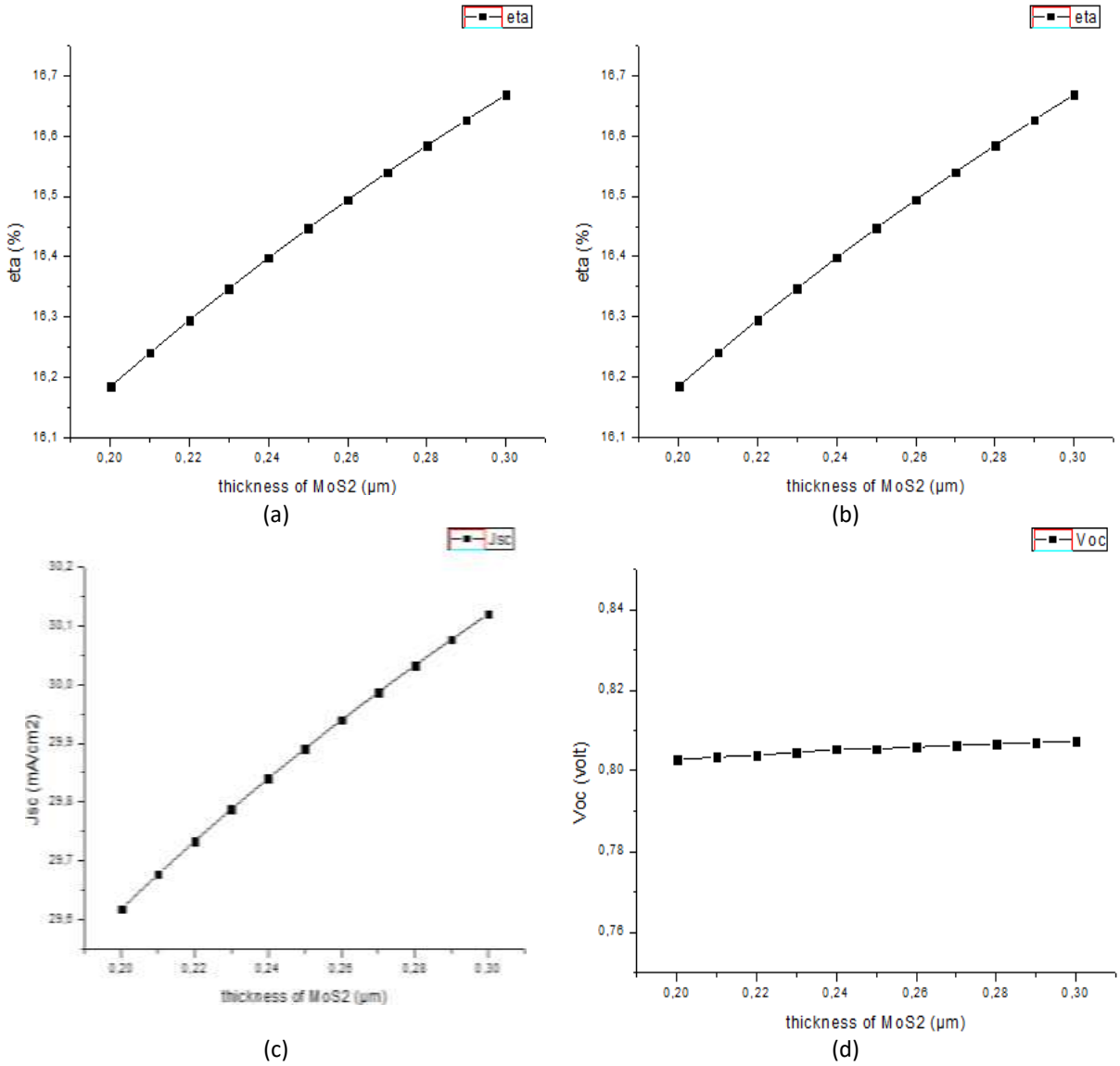

Fig. 4. Variation of cell efficiency, (a) eta, (b) FF, (c) Jsc and (d) Voc with interfacial layer

3.4 Examining the Impact Variation of Back Contact

In the intricate landscape of solar structures, the back metal contact stands out as another parameter of substantial technological importance, as thoroughly discussed in previous studies [18,21,22]. Within the confines of Figure 5, our investigation delved into the nuanced dynamics of the electron work value, spanning the range of 5–6 eV, with a keen focus on unraveling its consequential impact on the output performance of the envisioned solar cell. Remarkably, our

scrutiny unearthed a discernible pattern, both open circuit voltage and efficiency experienced an almost linear upswing within the 5.0–5.5 eV bracket. A subsequent phase revealed these pivotal output parameters showcasing a relatively stable evolution between 5.5 eV and 6.0 eV. The intricacies elucidated by these findings have far-reaching implications for the optimization of solar cell performance. Drawing cohesive conclusions from our simulation results, it becomes evident that platinum, boasting an electron work value of 5.7 eV, emerges as the most judicious choice to supplant molybdenum as the metal back contact. This nuanced understanding of the interplay between the electron work value and solar cell performance not only underscores the significance of the back metal contact but also propels us towards more informed and effective choices in the quest for enhanced solar energy technologies.

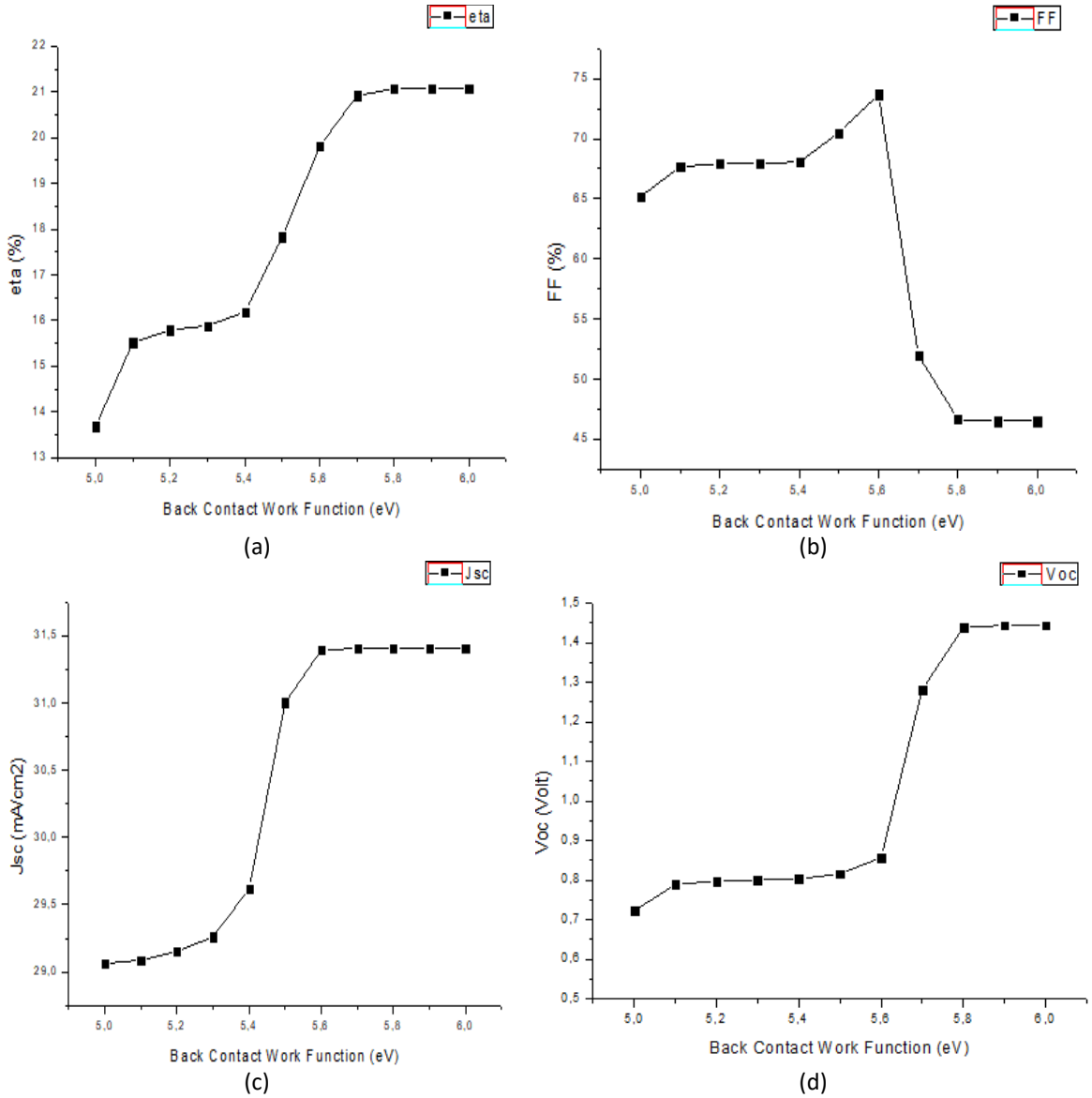

Fig. 5. Variation of cell efficiency, (a) eta, (b) FF, (c) Jsc and (d) Voc with back contact work function (ev)

4. Conclusion

In conclusion, the article provides a comprehensive analysis of CZTS solar cells, elucidating various factors that influence their performance. Through meticulous experiments, researchers explore the

intricate relationship between the thickness of the absorbing layer and key photovoltaic parameters. By varying this thickness within a 400 nm range, a compelling trend emerges: thicker absorbing layers exhibit significant improvements in Voc, Jsc, FF, and PCE. This enhancement is attributed to increased photon absorption, leading to a heightened production of electron-hole pairs within the device.

Furthermore, the study highlights the impact of temperature fluctuations on solar cell performance, particularly emphasizing the sensitivity of MoS_2, the hole transport layer, to thermal variations. This sensitivity manifests in fluctuations in Voc and Jsc, underscoring the importance of effective thermal management strategies in solar cell design and operation. Additionally, the investigation extends to optimizing back surface fields (BSF) and selecting back metal contact materials. By adjusting the thickness of MoS_2 as the BSF layer, a continuous improvement in PCE is observed, attributed to enhanced photon reflection. PCE = 16.6684%, FF = 68.5442%, Jsc = 30.11985173 mA/cm^2 and Voc = 0.807367 V.

Moreover, the detailed examination of the electron work function reveals intriguing insights, with platinum emerging as a preferable choice over molybdenum for the back metal contact. This nuanced understanding of material selection underscores the crucial role of engineering precise interfaces within the solar cell structure to optimize performance.

Overall, the article offers a wealth of details on the complex interactions influencing the behavior of CZTS solar cells. By unraveling these intricacies, the study not only advances our fundamental understanding of photovoltaic technology but also provides practical recommendations for enhancing device performance in real-world applications. These promising conclusions pave the way for the continued development of efficient and sustainable solar energy systems to address global energy challenges. The results obtained for the MoS_2 interface reinforce these conclusions, highlighting its crucial role in optimizing the performance of CZTS solar cells.

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