

Numerical Investigation of High Efficiency Cu_2SnSe_3 Thin Film Solar Cell with a Suitable ZnSe Buffer Layer Using SCAPS 1D Software

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ABSTRACT

As the world's energy demand continues to grow, thin-film solar cells are poised to play an increasingly important role in meeting that demand. In this research, we have proposed and simulated a high-efficiency Cu_2SnSe_3 -based thin film solar cell structure using a solar cell capacitance simulator (SCAPS-1D) software. The numerical performance of Cu_2SnSe_3 thin films solar cell with ZnO:Al as the electron transport layer (ETL), ZnSe as the buffer layer, SnS as the hole transport layer (HTL), Ag as the front and Ni as the back contact with the structure ($\text{Ag/ZnO:Al/Cu}_2\text{SnSe}_3/\text{SnS/Ni}$) has been studied. This simulation intended to investigate the effect of the ZnO:Al electron transport layer and SnS hole transport layer on the performance of the proposed solar cell. The device was optimized concerning the thickness, temperature, series and shunt resistance, donor density of the Electron transport layer, back contact metal work function, and acceptor density of the Cu_2SnSe_3 -based thin film solar cell. The thickness of the ETL, buffer, absorber, and HTL was optimized to 0.2 μm , 0.05 μm , 1.5 μm , and 0.1 μm , respectively. The proposed cadmium-free Cu_2SnSe_3 thin films solar cell exhibited a conversion efficiency of 31.04%, V_{OC} of 1.08 V, J_{SC} of 34.11 mA/cm^2 , and FF of 83.84%. As a result, due to its low cost, earth-abundant, non-toxicity, and high efficiency, the suggested Cu_2SnSe_3 -based solar cell may be an attractive candidate for thin film solar cells.

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1. INTRODUCTION

The scarcity of natural energy resources and the environmental damage caused by conventional energy, the need for alternative energy sources has recently surged significantly. Consequently, reducing energy use and safeguarding the environment has increasingly drawn attention worldwide. Solar energy is the most abundant, consistent, and environmentally friendly alternative energy source and the least expensive. The technology for thin film solar cells offers a more significant benefit in terms of lowering the consumption of raw materials, omitting energy-intensive production procedures, and improving performance stability at actual working temperatures. However, crystalline silicon-based solar cells have the highest efficiency of all wafer-based technologies, at 26.7% (for single cells) and 24.4% (for modules) [1]. The first-reported thin film solar cells are single-junction cuprous sulfide-cadmium sulfide

($\text{Cu}_2\text{S}/\text{CdS}$) solar cells, with a PCE of about 9.1%. However, the long-term performance is compromised by copper diffusion into the CdS matrix and doping of the CdS layer, leading to the rejection of further research activities on $\text{Cu}_2\text{S}/\text{CdS}$ solar cells [2], [3].

Recently, ternary and quaternary semiconductor compounds, such as Cu_2SnS_3 (CTS) and Cu_2SnSe_3 (CTSe), have been reported as desirable materials for optoelectronics applications [4]. Due to its appropriate optoelectronic properties, the ternary chalcogenide-based semiconductor Cu_2SnSe_3 has been proposed as a contender for the bottom material of earth-abundant, affordable, and current photovoltaic absorbers [5]. Cu_2SnSe_3 has a high light absorption coefficient (10^4 – 10^5 cm^{-1}) [1]. A recently published research paper on Cu_2SnS_3 -based solar cells with a ZnS buffer layer exhibits the best efficiency of 17.0% [5]. Another research work published Cu_2SnS_3 -based solar

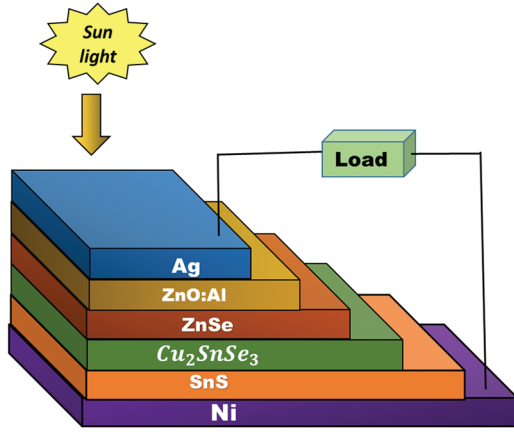


Fig. 1. Schematic diagram of the proposed Cu₂SnSe₃ thin film solar cell having the structure of Ag/ZnO:Al/ZnSe/Cu₂SnSe₃/SnS/Ni.

cell with a CdS buffer layer showed a power conversion efficiency of 9.87% [6]. An experimental research paper published Cu₂SnSe₃-based solar thin film solar cells achieved maximum efficiency of 1.17% [7]. In a previous simulation, work with Ni/SnS/Cu₂SnSe₃/TiO₂/ITO/Al structures attained an efficiency of up to 27% [1]. However, the International Agency for Research on Cancer and the National Institute for Occupational Safety and Health both classify TiO₂ as an occupational carcinogen and “possibly carcinogenic to humans” based on experimental data from animal inhalation experiments [8].

In our research, we have proposed a Cu₂SnSe₃-based thin film solar cell structure (Ag/ZnO:Al/Cu₂SnSe₃/SnS/Ni) with ZnSe and SnS as buffer layer materials and hole transport layers. The novelty of this research is that in this reserach, we used nontoxic ZnSe as a buffer layer material and achieved an efficiency of 31%. Hence, due to its environmentally friendly nature, ZnSe might be a viable substitute for toxic CdS [9], [10]. Since ZnSe has a wider band gap than CdS, its typical absorption range is closer to 450 nm than that of CdS, which is close to 500 nm. The wide-band-gap buffer material provides high UV absorption and optical transparency in visible and IR regions [11], [12]. As a result, using ZnSe as a buffer material can also reduce the loss of those useful visible-range photons, which can produce charge carriers that may contribute to the photocurrent. ZnSe can be synthesized by thermal evaporation, spray pyrolysis, chemical bath deposition, electro-deposition, etc. [13], [14].

In this study, we have also used SnS as a hole transport layer. SnS has a bandgap energy of 1.07 eV to 1.6 eV, an optical absorption coefficient of up to 10⁴ cm⁻¹, hall mobility of up to 100 cm²/Vs, and a majority carrier concentration of 10¹⁵ cm⁻³ to 10¹⁸ cm⁻³. SnS is an attractive hole transport layer material due to its excellent electrical and optical properties, low toxicity, earth abundance, cost-effectiveness, and stability [15]. In addition, to improve the efficiency, several ETL layer materials, including ZnO:Al, ITO, CdS, and CeO₂, have been tried with absorber layers [7], [16]–[21]. A few HTL layer materials such as SnS, Co-P₃HT, Niox and Spiro-OMeTAD were employed with a ternary chalcogenide-based absorber layer [22], [18]–[20]. We achieve the highest efficiency and optimal performance

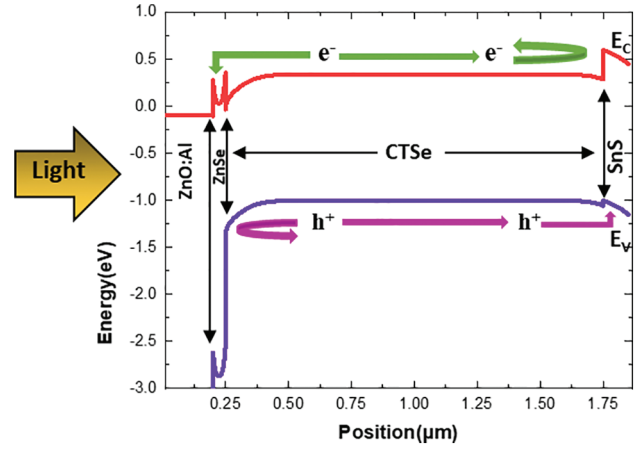


Fig. 2. Energy band diagram of Cu₂SnSe₃ solar cell.

for the absorber layer Cu₂SnSe₃ when ZnO:Al is used as an electron transport layer (ETL) and SnS as a hole transport layer.

2. DEVICE ARCHITECTURE AND SIMULATION

The photovoltaic cell was created and its performance was examined using the SCAPS-1D software application. Researchers from the Electronics and Information Systems (ELIS) Department of the University of Gent in Belgium created the numerical simulation program SCAPS [18]. We chose SCAPS because it outperforms other solar device simulator software and because its simulation findings closely match those of current experiments.

For the free electrons and holes in conduction and valence bands, Poisson's equation and the continuity equation are used. The electron and hole continuity formulas are:

$$\frac{dJ_n}{dx} = G - R \quad (1)$$

$$\frac{dJ_p}{dx} = G - R \quad (2)$$

where R is the recombination rate, G is the generation rate, and J_n and J_p are the respective electron and hole current densities.

The Poisson equation is:

$$\frac{d^2\psi(x)}{dx^2} = \frac{e}{\epsilon_0\epsilon_r} (\rho(x) - n(x) + N_D - N_A + \rho_p - \rho_n) \quad (3)$$

where ψ is the electrostatic potential, e is the electrical charge, ϵ_r is the relative permittivity, and ϵ_0 is the vacuum permittivity, p and n are concentrations of holes and electrons, N_D are the charged impurities of the donor type, and N_A are the acceptor type, and ρ_p and ρ_n are the distributions of holes and electrons, respectively [23], [24]. Table I shows the physical parameters of each layer used in the simulation: ZnO:Al, ZnSe, Cu₂SnSe₃, and SnS.

TABLE I: PHYSICAL PARAMETERS OF EACH LAYER USED IN THE SIMULATION WERE ZnO:Al , ZnSe , Cu_2SnSe_3 , SnS (VB = VALENCE BAND, CB = CONDUCTION BAND)

Parameters (unit)	ZnO:Al [7], [16]	ZnSe [25], [26]	Cu_2SnSe_3 [1], [4]	SnS [1]
Thickness (μm)	0.2	0.05	1.5	0.1
E_g (eV)	3.3	2.9	1.34	1.6
X (eV)	4.4	4.02	4.41	4.1
ϵ_r	9	10	10	13
N_c (cm^{-3})	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}	1.18×10^{18}
N_b (cm^{-3})	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	4.46×10^{18}
μ_e ($\text{cm}^2/\text{V}\cdot\text{s}$)	1.0×10^2	2.5×10^1	100	15
μ_h ($\text{cm}^2/\text{V}\cdot\text{s}$)	2.5×10^1	1×10^2	25	100
N_D (cm^{-3})	1×10^{20}	1×10^{18}	0	0
N_A (cm^{-3})	0	0	1×10^{16}	1×10^{16}

3. RESULTS AND DISCUSSIONS

3.1. J-V Characteristics of Cu_2SnSe_3 Solar Cell

The thickness of the absorber layer can significantly impact the J-V curve and overall solar cell performance. Fig. 3 shows the J-V characteristics of the schematic Cu_2SnSe_3 -based thin film solar cell by varying the thickness of the absorber layer. The absorber layer thickness varied from 0.1 μm to 2.5 μm . Efficiency also increased from 14.68% to 31.32%. A thicker absorber layer tends to absorb more light, resulting in a higher number of electron-hole pairs generated. As a result, the photocurrent in the J-V curve will increase with increasing absorber layer thickness [27].

3.2. Quantum Efficiency of Cu_2SnSe_3 Solar Cell

Quantum efficiency (QE) refers to the ability of a solar cell to convert incident photons into electrical charge carriers (electrons and holes). It is typically represented as a percentage and varies with the wavelength of light. Fig. 4 shows the relationship between quantum efficiency and wavelength for absorber layer with thickness varying from 0.1 to 2.5 μm . Photons are more deeply absorbed at wavelengths below 900 nm. This is because photons of longer wavelengths (>900 nm) were absorbed far from the depletion area, deep down in the absorber layer. The quantum efficiency of a photovoltaic cell determines how efficiently it can capture carriers from incoming photons of certain energy [28].

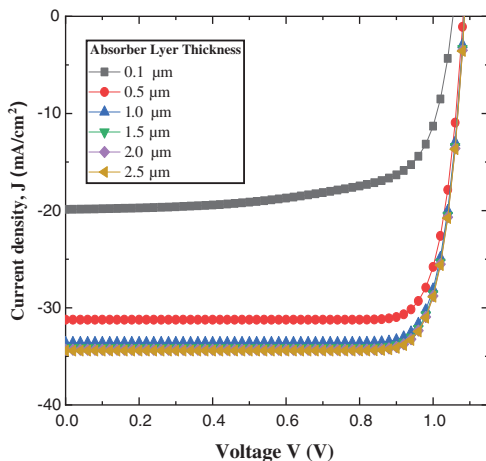


Fig. 3. J-V characteristics of the varying absorber layer thickness.

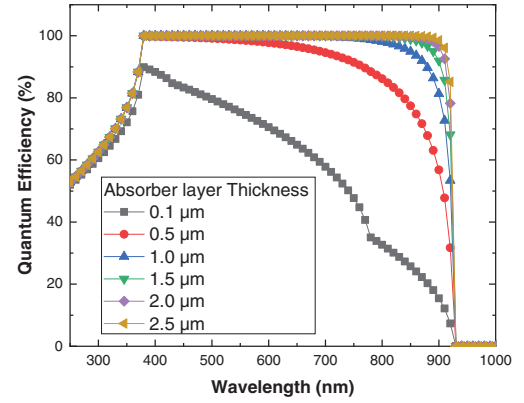


Fig. 4. Quantum efficiency vs. wavelength for absorber layer thickness.

3.3. Absorber Layer Thickness Variation of Cu_2SnSe_3 Solar Cell

Fig. 5 illustrates how the thickness of the absorber layer impacts the output parameters V_{OC} , J_{SC} , FF, and efficiency. The ZnSe buffer layer thickness was fixed at 0.05 μm , the absorber layer Cu_2SnSe_3 thickness was changed from 0.1 to 2.5 μm and the values of the SnS (HTL) 0.1 μm , ZnO:Al (ETL) 0.2 μm , Ag and Ni were as front and back contact at the temperature of 300 K. When the active layer thickness is 0.1 μm the obtained values of V_{OC} of 1.05 V, J_{SC} of 19.87 mA/cm^2 , FF of 70.07%, and efficiency of 14.69%. And when the thickness is 2.5 μm obtained V_{OC} of 1.08 V, J_{SC} of 34.42 mA/cm^2 , FF of 83.83% and efficiency of 32.33% shown in Fig. 5. The simulation findings show that all parameters, such as V_{OC} , J_{SC} , FF, and efficiency, increase as the absorber layer thickness increases. More electron-hole pairs are formed, and more photons are absorbed by an absorber layer that is thicker than one that is thinner [28].

3.4. Acceptor Density Effect on the Absorber Layer

The acceptor density on the absorber layer has a significant effect on the performance of solar cells. The acceptor density effect on the absorber layer (Cu_2SnSe_3) is shown in Fig. 6. From 1×10^{12} to $1 \times 10^{18} \text{ cm}^{-3}$, the acceptor density of the Cu_2SnSe_3 layer has changed. Up until $1 \times 10^{15} \text{ cm}^{-3}$, every output result stayed the same. V_{OC} , J_{SC} , FF and efficiency rise with acceptor density from 1×10^{15} to $1 \times 10^{18} \text{ cm}^{-3}$ and are acquired as 1.13 V, 34.17 mA/cm^2 , 88.37% and 34.27%. But J_{SC} at $1 \times 10^{15} \text{ cm}^{-3}$

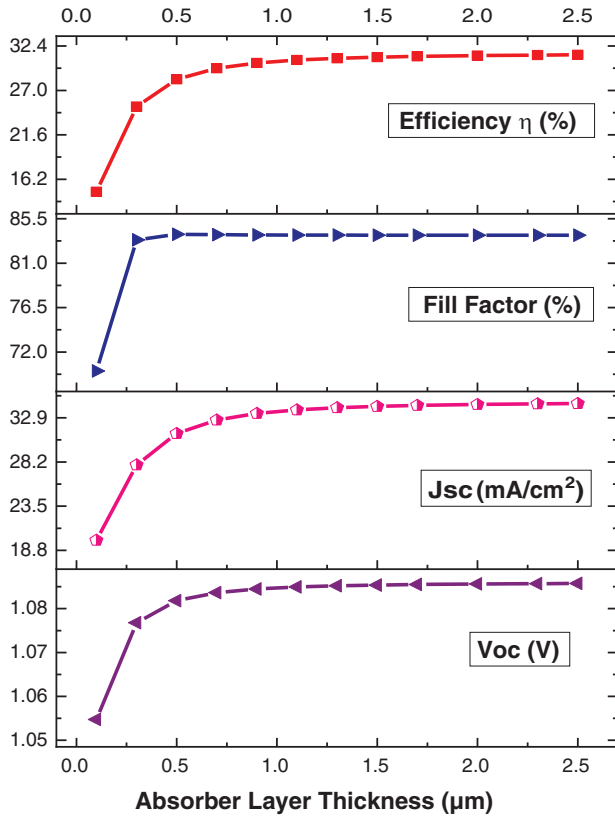


Fig. 5. Absorber layer thickness variation of Cu_2SnSe_3 based solar cell.

decreases to 34.10 mA/cm^2 . The open circuit voltage rises due to improved reverse saturation current brought on by increased doping concentration, which boosts FF and conversion efficiency [29].

3.5. Temperature Effect on the Cu_2SnSe_3 Solar Cell

The performance of photo voltaic cells is significantly influenced by temperature rise [30]. Temperature changes can influence various solar cell parameters, affecting its electrical characteristics and overall energy conversion efficiency. With an absorber layer thickness of $1.5 \mu\text{m}$ and a $0.05 \mu\text{m}$ buffer layer, we have changed the temperature from 250 K to 425 K as shown in Fig. 7. In this temperature changes, V_{OC} varied from 1.18 to 0.76 V , J_{SC} changes 34.11 to 34.12 mA/cm^2 , fill-factor varies 83.03% to 79.86% and efficiency varies 33.53% to 20.74% . As the temperature increases, the V_{OC} decreases. This is due to an increased intrinsic carrier concentration of the semiconductor material with temperature, leading to a more significant recombination of charge carriers and reducing the voltage potential across the cell. Consequently, there is an increase in the rate of recombination between electrons and holes. So the values of V_{OC} , FF and efficiency decrease with increasing temperature [31].

3.6. Back-Contact Effect on the Cu_2SnSe_3 Solar Cell

The back-contact work function is essential in Cu_2SnSe_3 -based solar cells. The work function of the device ranges from 5.1 to 5.65 eV and uses a variety of back contact materials, including Pt, Ni, Au, and Pd. When back-contact was varying the front contact was 4.73 eV (Ag) fixed with the absorber layer (Cu_2SnSe_3) and buffer

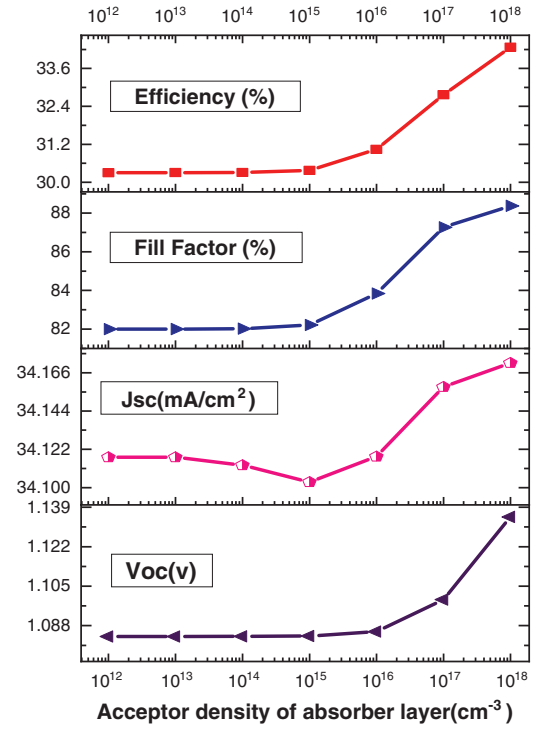


Fig. 6. Acceptor density effect on the Cu_2SnSe_3 based solar cell.

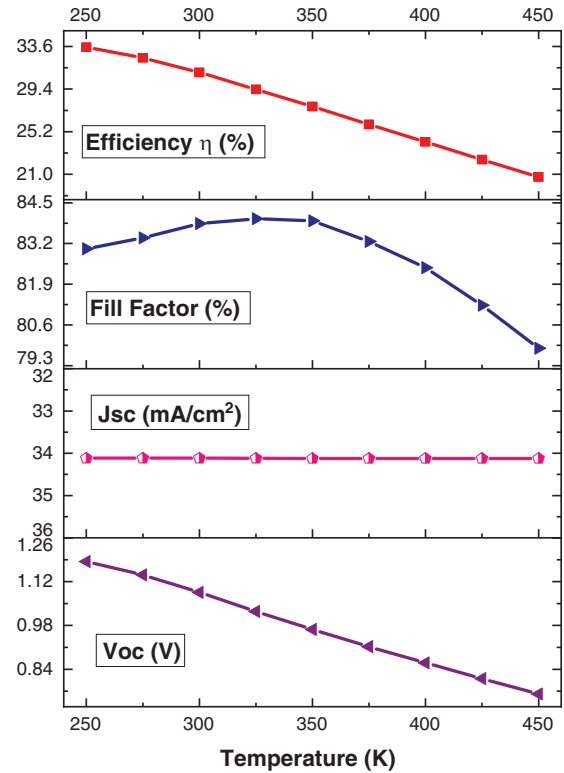
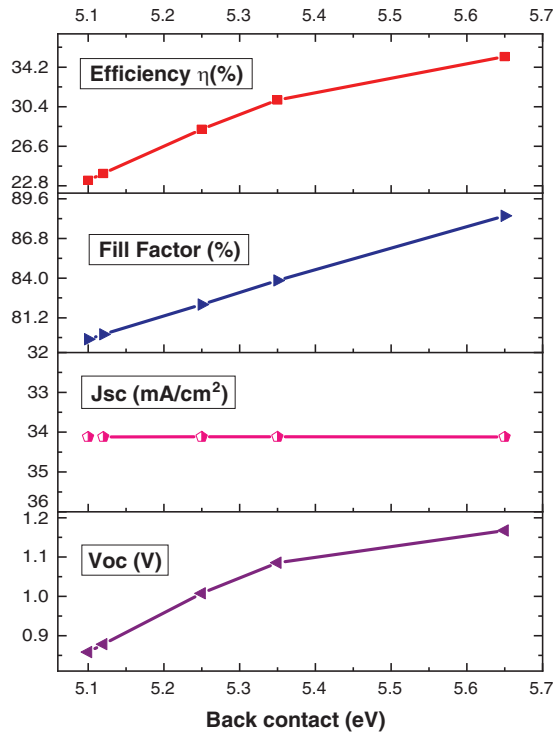


Fig. 7. Temperature effect on the Cu_2SnSe_3 based solar cell.

layer (ZnSe) thickness $1.5 \mu\text{m}$ and $0.05 \mu\text{m}$. As shown in Fig. 8 the V_{OC} , FF, and efficiency increased as the work function increased. As with the work function J_{SC} stays stable, in the earlier research a similar outcome for J_{SC} was also discovered [32]. Due to the significant barrier produced by the materials with a reduced work function on the back side, the hole cannot be transported from the

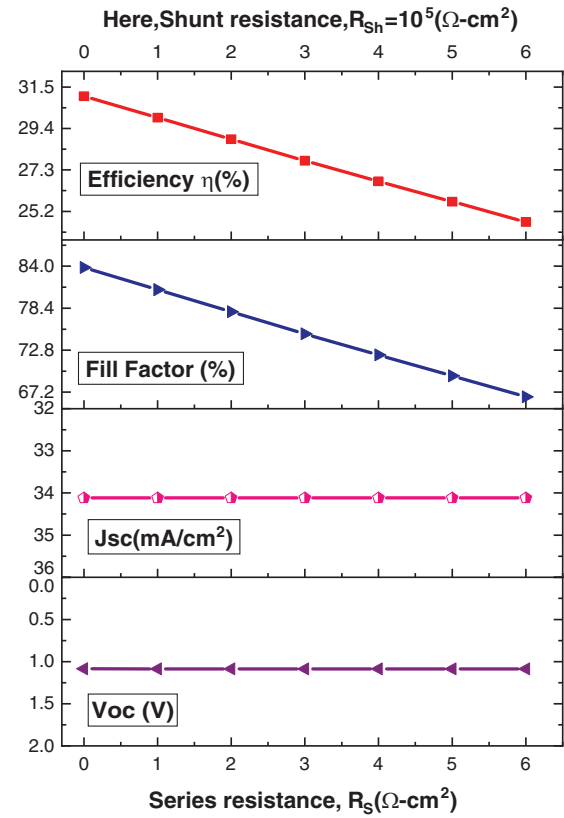
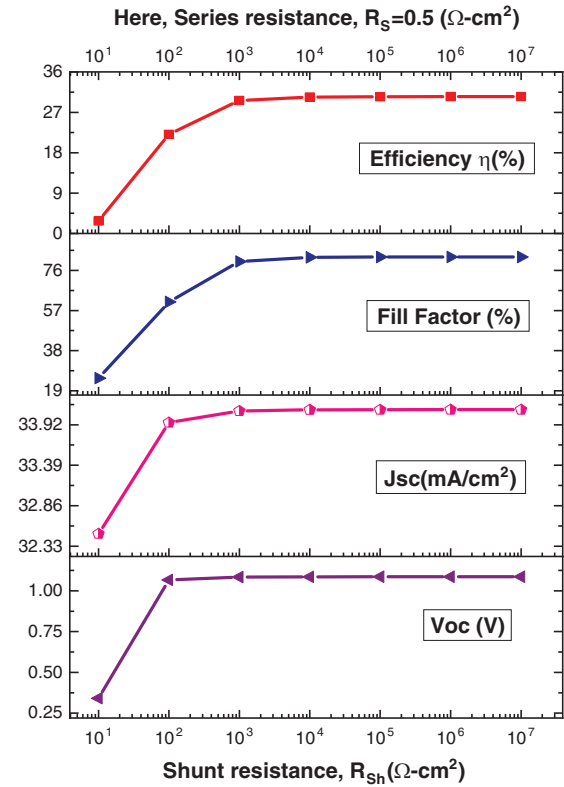
Fig. 8. Back-contact effect on the Cu_2SnSe_3 based solar cell.

absorber to the back contact, which results in poor solar output [17].

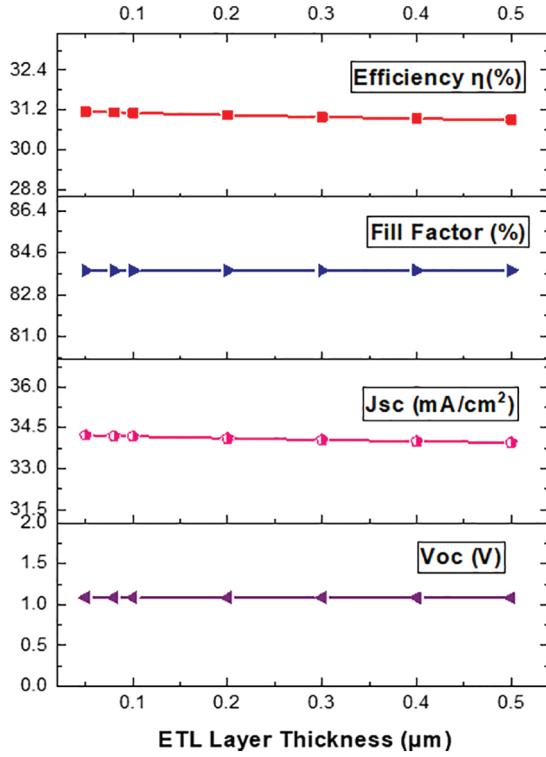
3.7. Series and Shunt Resistance Effect on Cu_2SnSe_3 Solar Cell

The impact of series (R_S) and shunt (R_{Sh}) resistance on the V_{OC} , J_{SC} , FF, and efficiency of ternary chalcogenide-based solar cells has been investigated [32]. Series resistance (R_S) is the total resistance offered by the electrical contacts and the semiconductor material in a solar cell. It is called “series” resistance because it is in series with the current path of the solar cell. Keeping R_{Sh} at $10^5 \Omega \text{ cm}^2$, the performance of the series resistance is investigated by changing R_S from 0 to $6 \Omega \text{ cm}^2$. As shown in Fig. 9, V_{OC} and J_{SC} remained essentially unchanged, but FF and efficiency decreased. As series resistance rises from 0 to $6 \Omega \text{ cm}^2$, efficiency decreased by 31.03% to 24.65%. When the solar cell generates electricity, some electrical energy dissipates as heat in the series resistance due to the voltage drop across it. This reduces the voltage available to the external load, resulting in a lower output voltage from the solar cell. As a result, the overall efficiency of the solar cell decreases [17].

As illustrated in Fig. 10, the Shunt resistance performance is investigated by altering R_{Sh} from 10^1 to $10^7 \Omega \text{ cm}^2$ while keeping R_S constant at $0.5 \Omega \text{ cm}^2$. Shunt resistance (R_{Sh}) represents the leakage current path in a solar cell. It is called “shunt” resistance because it provides an alternative current way parallel to the solar cell’s intended current direction. The experimentally determined series resistance of the thin film solar cell is extremely similar to the desired series resistance value in the current study [33]. All parameter values increase along with shunt resistance. Its efficiency increases by 2.77% to 30.49% when R_{Sh} increases to a higher value. FF, J_{SC} , and V_{OC}

Fig. 9. Series resistance effect on Cu_2SnSe_3 based solar cell.Fig. 10. Shunt resistance effect on Cu_2SnSe_3 based solar cell.

are observed at 24.99%, 32.49 mA/cm^2 and 0.34 V when R_{Sh} $10^1 \Omega \text{ cm}^2$, and these output parameters varied to 82.35%, 34.11 mA/cm^2 and 1.08 V when R_{Sh} $10^7 \Omega \text{ cm}^2$. These results demonstrate that series and shunt resistances greatly affect the performance of solar devices [34].

Fig. 11. ETL layer thickness effect on Cu_2SnSe_3 based solar cell.

3.8. ETL and HTL Layer Thickness Effect on Cu_2SnSe_3 Solar Cell

In this simulation work, we use ZnO:Al as the electron transport layer (ETL). From Fig. 11, we can obtain solar cell output parameter values for V_{OC} , J_{SC} , FF and efficiency that are stable at the thickness of ZnO:Al 0.05 to 0.5 μm . Because the changes were so modest, the graph remained roughly steady as we increased the thickness. At the thickness of 0.05 μm solar cell output parameter values are V_{OC} of 1.085536 V, J_{SC} of 34.23167439 mA/cm^2 , FF of 83.8316% and efficiency of 31.1516% and at the thickness of 0.5 μm variables are V_{OC} of 1.085161V, J_{SC} of 33.96253594 mA/cm^2 , FF of 83.8412% and efficiency of 30.8995%. The graph makes it obvious that the photovoltaic characteristics stay constant as the ETL's thickness varies; this means that the output of solar cells is not significantly affected by the ETL's thickness [17].

The structure was modeled to explore the simultaneous of the SnS layer varied from 0.1 to 0.6 μm . With increased HTL layer thickness, FF and efficiency increase, but V_{OC} and J_{SC} remain approximately stable. At the thickness of 0.1 μm FF of 83.83% and efficiency of 31.04% and at the thickness of 0.6 μm FF of 81.18% and efficiency of 34.71% effects of SnS HTL thickness. Fig. 12 shows the HTL layer thickness effect on Cu_2SnSe_3 solar cell. The thickness of the SnS layer varied from 0.1 to 0.6 μm . With increased HTL layer thickness, FF and efficiency increase, but V_{OC} and J_{SC} remain approximately stable. At the thickness of 0.1 μm FF of 83.83% and efficiency of 31.04% and at the thickness of 0.6 μm FF of 81.18% and efficiency of 34.71%.

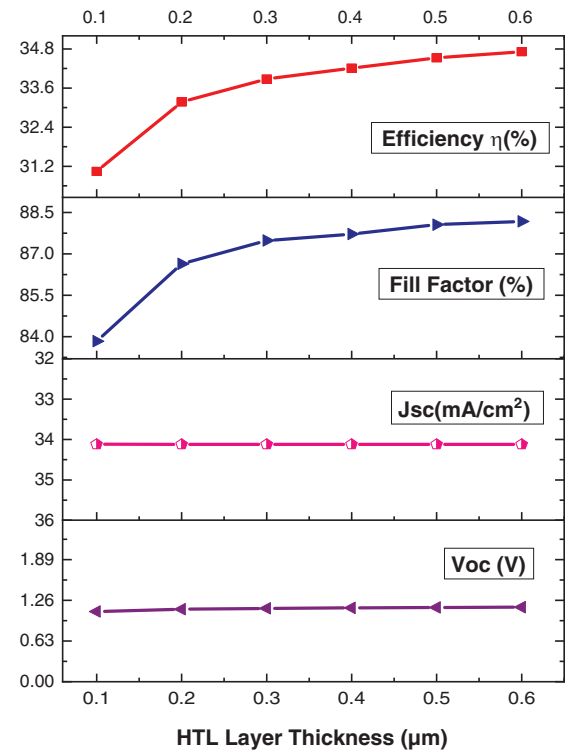
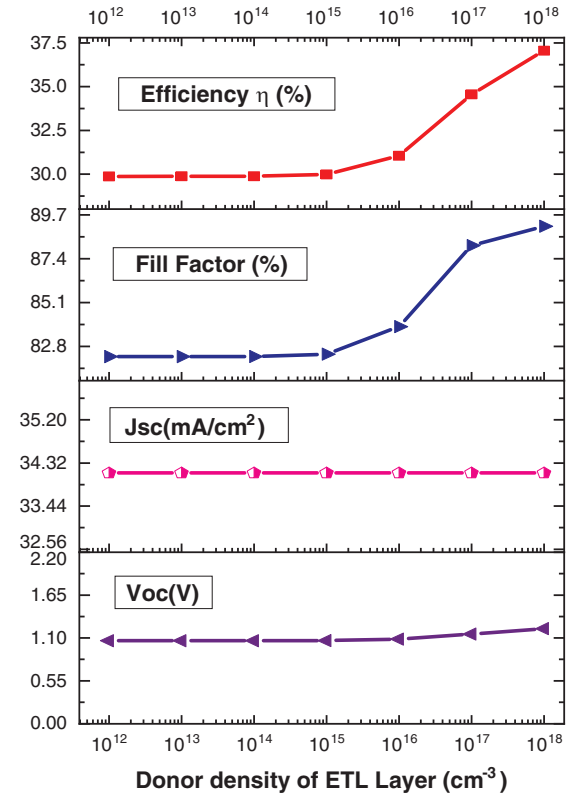
Fig. 12. HTL layer thickness effect on Cu_2SnSe_3 based solar cell.

Fig. 13. Donor density effect on the ETL layer.

3.9. Donor Density Effect on the ETL Layer

In order to examine the impact of the donor density of the ETL (ZnO:Al) on the functionality of the solar cell, the ETL layer donor density was adjusted 1×10^{12} to $1 \times 10^{18} \text{ cm}^{-3}$. Fig. 13 displays the performance metrics for the ETL, including V_{OC} , J_{SC} , FF, and efficiency of donor density. With the rise in ETL donor density, it is

discovered that V_{OC} and J_{SC} stay roughly steady. However, after $1 \times 10^{15} \text{ cm}^{-3}$ both the FF values and the efficiency began to rise. At $1 \times 10^{18} \text{ cm}^{-3}$ the donor density of ETL FF is 89.09% and efficiency 37.05%. A thin ETL layer is projected to result in high solar cell activity since it is assumed that less light would pass through the absorber through a thicker buffer layer, leading to a minimal current for inadequately create electrons and holes [35].

4. CONCLUSION

In this research, we have optimized the thickness, operating temperature, series, and shunt resistances of Cu₂SnSe₃ thin film solar cells using SCAPS-1D software. The optimum thicknesses of 1.5 μm , 0.05 μm , 0.2 μm and 0.1 μm are found for the Cu₂SnSe₃, ZnSe, ZnO:Al and SnS, respectively. The simulation revealed that the Cu₂SnSe₃-based thin film solar cell device's efficiency without the SnS hole transport layer was 22%. In this study, the efficiency of the solar cell is increased to 31.04% with the suggested innovative solar cell structure (Ag/ZnO:Al/Cu₂SnSe₃/ZnSe/SnS/Ni), and V_{OC} , J_{SC} , and FF are 1.08 V, 34.11 mA/cm², and 83.83%, respectively. For the proposed Cu₂SnSe₃-based solar cell, the temperature dependency performance metrics have also been investigated. These findings point to the possibility of using the p-type Cu₂SnSe₃ material as a viable absorber layer for use in the highly effective ternary chalcogenide based thin-film solar cell.

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