SCAPS-1D Study of SnS Absorber Based Solar Cell; Effect of Thickness and Bang Gap

Sunil Kumar[1], **Saurabh K Sengar**[2]

[1]Department of Physics, D. S. College, Aligarh, India-202001
Email: *sunildeswal484[at]gmail.com*

[2]Department of Physics, D. S. College, Aligarh, India-202001
Email: *saurabhhsengar[at]gmail.com*

Abstract: ***Tin Sulphide (SnS) is considered to be one of the best absorber materials in solar cell applications, due to its high absorption coefficient, optimal band gap, earth abundance and non-toxic nature. In this study the effect of SnS thickness and band gap on the solar cell performance has been studied in terms of efficiency, Voc, Jsc and FF. In the proposed structure Al/Zn(O,S)/SnS/MoO3/Au, Zn(O,S) has been used as an ETL, while MoO3 serves the purpose of HTL. It is found that on increasing the thickness, solar cell performance first increases and then decrease after 1.4 µm. Similarly, the solar cell attains a maximum efficiency at 1.3 eV. On using the optimized values of thickness and band gap, an efficiency of 27.1%, V_{oc} of 0.92 V, J_{sc} of 34.8 mAcm⁻² and FF of 84.9 % were obtained.***

Keywords: Tin Sulphide, Thin film solar cell, Zn (O, S), MoO3, Electron Transport Layer and Hole Transport Layer

1. Introduction

The continuously increasing global warming, due to the excessive use of coal and petroleum products, has forced the scientists to work on alternate energy materials. Solar energy is considered to be one of the best solutions in this direction, as it is easily and abundantly available in most parts of the earth. Solar energy can be harnessed using either the solar thermal or solar photovoltaics (PV). Although, now a days, 90% of solar energy is being harnessed using solar photovoltaics (PV), but the high cost of solar PV technologies is the main problem in their widespread adoption [1,2]. Therefore, it is crucial to device schemes that can lower the operational costs while achieving similar or higher power conversion efficiencies (PCE). It is now generally recognised that the most promising way to reduce production costs is to use thin films based on direct energy bandgap materials. Such layers need to be only a few microns thick to absorb all of the incident light, minimising material costs [1,2]. At present, cadmium telluride (CdTe) and copper-indium-gallium diselenide (CIGS) seem to be the most promising thin film solar cell materials. Although CdTe-based thin film solar cells have reported an efficiency of 18.7%, their toxic nature and the low abundance of the constituent elements, i.e., Cd, Te and Se in Earth's crust, limit their commercialisation at a larger scale like Si-based solar cells [3,4]. In the same manner, CIGS cells, which have an efficiency as high as 23.64% also suffer from the same problem [5]. Perovskite solar cells have been reported to have efficiencies greater than 25 % but their long-term stability in atmosphere is the main reason which prevents their large-scale use [6]. Therefore, researchers have focussed their attention towards solar cell materials that are nontoxic, highly abundant and stable in nature. In this regard, Tin Sulfide (SnS) is considered to be one of the best absorber materials due to its wide band gap, high absorption coefficient of light, superior electrical conductivity, non-toxicity, low cost, high natural abundance, thermal stability, durability and compatibility with other Materials. Moreover, due to a direct energy band gap of about 1.3 eV and a high optical absorption coefficient (> 10^4 cm^{-1}), only a few microns of SnS are needed to absorb all of the incident light [1,2]. Besides, SnS has a Hall mobility and tunable carrier densities of the order of 100 cm^2 Vs^{-1} or higher, and 10^{18} cm^{-3} [7–9]. In addition, SnS exhibits tunable conductivity, enabling both n-and p-type doping either by altering the stoichiometry of the compound or by extrinsic doping with suitable elements, e.g., Ag, Al, N and Cl [10,11].

Plenty of studies on SnS, using ETL and HTL have been reported with a decent efficiency [12–14]. This study proposes a novel, simple and non-toxic Al/Zn(O,S)/ SnS/ MoO_3/ Au device structure. This configuration utilizes Zn(O,S) as the electron transport layer which facilitates the flow of electron towards cathode while MoO_3 has been used as a hole transport layer which facilitates the flow of holes towards anode in addition to blocking the flow of electron towards anode. Numerical simulations using SCAPS-1D have been performed to study the effect of SnS absorber thickness and band gap on the solar cell parameters that include, power conversion efficiency, Voc, Jsc and FF. These simulations will guide the experimentalists to fabricate high efficiency SnS based solar cells.

Table 1: Material parameters used in SCAPS-1D simulation

Parameters (unit)	AZO [15]	Zn (O, S) [15]	SnS [15]	MoO_3 [15]
Thickness (µm)	0.2	0.05	0.9	0.05
Bandgap (eV)	3.3	2.7	1.31	3.08
Electron Affinity (eV)	4.45	4.3	4.2	2.3
Dielectric Constant	9	10	13	5.6
CB effective density of states (1/cm3)	2.2×10^{18}	2.2×10^{18}	1.18×10^{18}	1.19×10^{19}
VB effective density of states(1/cm3)	1.8×10^{19}	1.8×10^{19}	4.76×10^{18}	3.00×10^{19}
μ_e (cm^2/V·s)	100	100	130	29
μ_h (cm^2/V·s)	25	25	4.3	16
Doping Type	n-type	n-type	p-type	p-type
Doping Concentration (cm^{-3})	1×10^{18}	1×10^{17}	1×10^{16}	1×10^{17}
Defect Density (cm^{-3})	1×10^{14}	1×10^{14}	1×10^{15}	1×10^{15}

2. Device Structure and Simulation Details

The schematic diagram of the proposed solar cell device structure is shown in Fig. 1. It is evident that, Gold (Au) and Aluminum (Al) have been used as the back and front contacts. Tin Sulphide (SnS) is the main absorber layer. In this structure Zn(O,S) acts as an electron transport layer while MoO3 acts as a hole transport layer.

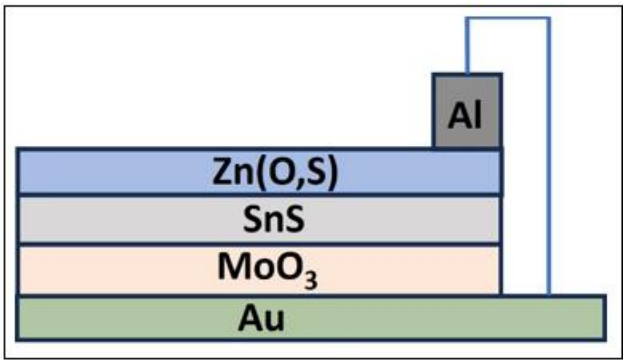

Figure 1: Schematic diagram of the SnS absorber-based thin film solar cell

Numerical simulations were performed using the SCAPS 3311 software developed by the Electronics and Information Systems (EIS) Department at the University of Gent, Belgium. This software basically solves the Poisson equation with appropriate boundary conditions reflective of the device contacts and predicts the device performance such as current–voltage behaviour under illumination. While performing the simulations, standard illumination conditions (AM1.5G, 1000 W/m^2) at a fixed temperature of 300 K, assuming a device area of 1 cm^2, were chosen. The various parameters used in simulations were selected from the earlier reported literature and are highlighted in Tables 1. The metal contacts are assumed to form Ohmic contacts with Zn(O, S) and MoO$_3$. To study the effect of thickness and band gap on the solar cell performance, the thickness and band gap of the SnS absorber layer were varied from 0.5 to 5 um and 1.2 to 1.6 eV, respectively.

3. Results and Discussion

3.1 Effect of the thickness of absorber layer

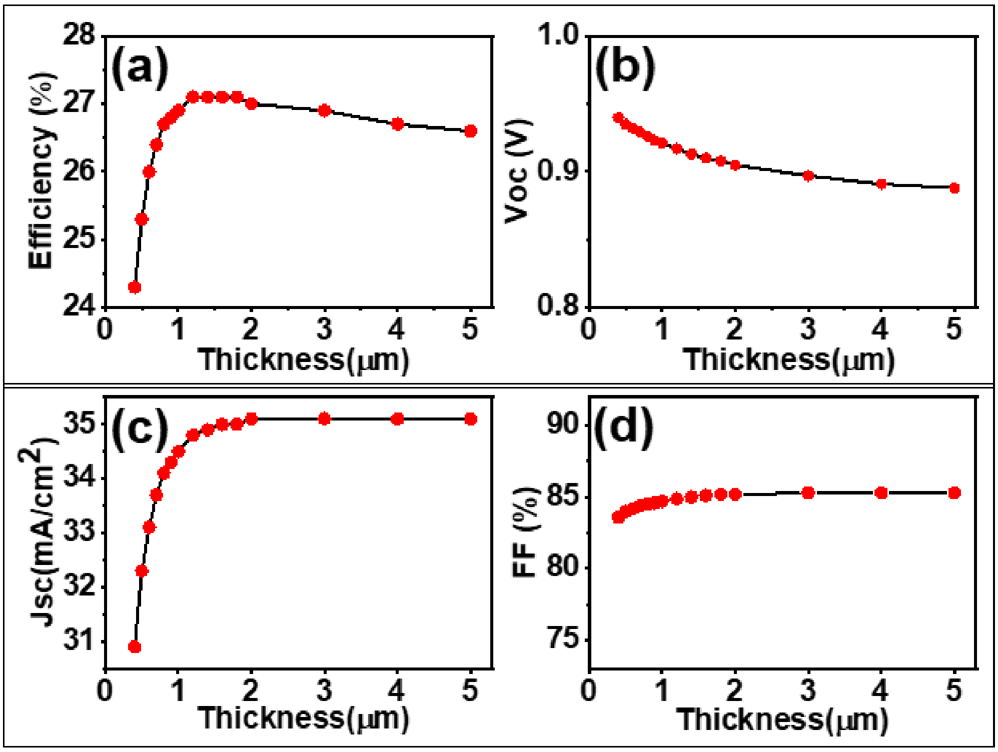

Figure 2: Effect of SnS thickness variation on (a) Efficiency (η), (b) V_{oc}, (c) J_{sc} and (d) FF

The thickness of the absorber layer is a critical parameter in in designing the photovoltaic devices which significantly influences both cost and performance. An ideal thickness must maximize light absorption and charge carrier generation while minimizing internal recombination losses. This study investigates the impact of the variation in absorber thickness from 0.4 to 5.0 µm while keeping all other device parameters constant. The corresponding changes in efficiency (η), V_{oc}, J_{sc}, and FF are shown in Fig. 2. As the thickness increases from 0.40 µm to 1.2 µm the efficiency increases to a peak value of 27.1% from 24.3%. This improvement is mainly due to the corresponding increase in J_{sc} , which increases from 30.9 to 34.5 mAcm^{-2}, on increasing the thickness from 0.40 µm, to 1.2 µm. This increase in J_{sc} reflects stronger light absorption and greater photogenerated carrier density in the thicker SnS layer. In this range, increasing the absorber thickness directly benefits the current generation. However, once the absorber thickness exceeds 1.8 µm, the gain begins to level off. It can be observed form Fig. 2c that beyond 1.8 µm the photocurrent saturates which indicates that most incident photons are already absorbed. Unlike J_{sc} and efficiency, V_{oc} gradually decreases from 0.94 V to 0.89 V on increasing the thickness. This gradual decrease in V_{oc} can be attributed to increased bulk recombination, as carriers need to travel longer distances to reach the contacts. As shown in Fig 2d. the fill factor shows an initial improvement before plateauing at 85.3%, which shows that charge carriers move through the device without recombining. Overall, a SnS thickness of about 1.4 µm offers the optimal balance between strong absorption and efficient carrier collection, giving $\eta \approx 27.1\%$, $V_{oc} \approx 0.91$ V, $J_{sc} \approx 34.9$ mAcm^{-2}, and $FF \approx 85\%$. These trends align with earlier simulation studies on SnS thin-film solar cells, where Mekhbi et al. and Umar et al. highlighted a thickness-dependent trade-off between carrier generation and recombination losses [18,19]. Both the reports suggest that a moderate absorber thickness of 1–2 µm yields the best efficiency balance, providing practical design guidance despite the ideal nature of simulation results.

3.2 Effect of band gap variation

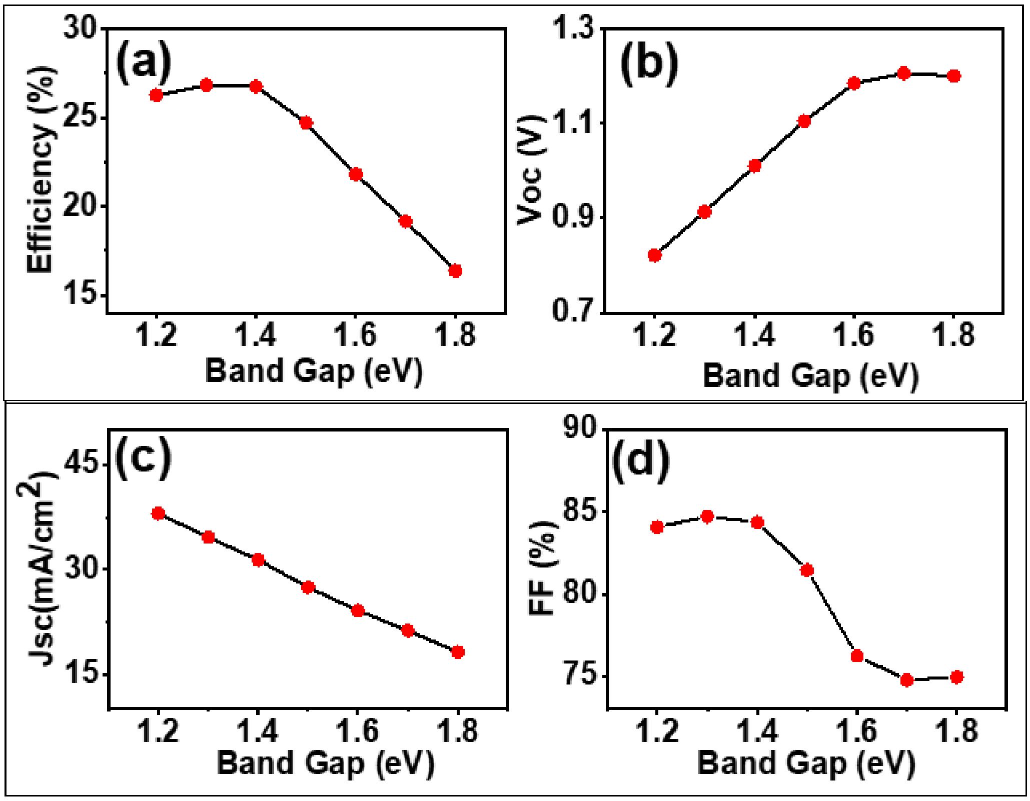

Figure 3: Effect of SnS band gap variation on (a) Efficiency (η), (b) V_{oc}, (c) J_{sc} and (d) Fill factor

The band gap of the absorber layer is a critical factor in determining the ability of a solar cell to harvest the solar energy. A narrow band gap allows for the absorption of a wider spectrum of photons but results in lower output voltage. Conversely, a wide band gap increases voltage but limits the number of photons that can be absorbed. This section analyses these trade-offs to identify the ideal band gap for maximum performance. The impact of band gap variation on the photovoltaic performance of the solar cell in terms of η, V_{oc}, J_{sc} and FF is shown in Fig. 3. The band gap was varied from 1.2 to 1.8 eV, which is well justified by the previous experimental reports [20,21]. As the band gap increases, a clear trade-off between photocurrent generation and voltage output can be observed from Fig. 3. As the band gap increases from 1.2 to 1.3 eV, efficiency rises from 26.3% to a maximum of 26.8%. This rise in efficiency is due to an increase in V_{oc} (from 0.82 V to 0.91 V) accompanied by a marginal decrease in J_{sc} (from 38.0 to 34.7 mA cm^{-2}). The observed increase in V_{oc} is expected, as it is fundamentally limited by the band gap of the absorber material. A larger gap reduces thermal recombination and allows for a higher potential difference. The decrease in J_{sc} on increasing the band gap indicates a reduction in absorption, because a wider band gap means the material can only absorb higher-energy photons, effectively "missing" a large portion of the solar spectrum's infrared and visible light. The fill factor remains almost constant between band gap values of 1.20 to 1.40 eV, which indicates that series resistance, junction quality, and charge-transport processes are largely insensitive to band-gap changes in this range. On increasing the band gap beyond 1.3 eV, η begins to decrease gradually due to reduction in FF and J_{sc}, despite a continued increase in V_{oc}. At 1.8 eV efficiency η drops to 16.4%, V_{oc} increases to 1.2 V, whereas, J_{sc} and FF drops to 18.2 mA cm^{-2} and 75%., respectively. It is clear from the Fig. 3, that beyond 1.4 eV, the loss in photocurrent and FF clearly outweighs the voltage gain, leading to an overall efficiency decrease. These findings indicate that an optimal SnS bandgap near 1.3 eV, balances high J_{sc}, elevated V_{oc}, and stable FF maximizes efficiency at 26.8%. Beyond 1.3 eV, the marginal voltage gain fails to offset reduced FF and spectral current losses. This behaviour aligns with detailed-balance theory for direct-gap absorbers under AM1.5G illumination [15].

4. Conclusion

The present investigation focused on optimizing the thickness and band gap of the Tin Sulphide (SnS) absorber layer to achieve maximum efficiency of the structure Zn(O,S)/SnS/MoO$_3$. The results demonstrate a critical trade-off between light absorption and carrier recombination. Increasing the SnS thickness initially boosts efficiency due to enhanced photon absorption and current generation; however, beyond 1.8 μm lead to a decline in open-circuit voltage and efficiency due to increased bulk recombination. An optimal thickness of approximately **1.4 μm** was identified, yielding an efficiency of **~27.1%**. Furthermore, the band gap analysis revealed that a value of **1.3 eV** provides the best balance between voltage gain and spectral absorption. Increasing the band gap beyond **1.3 eV** results in significant losses in J_{sc} and FF that outweigh any gains in V_{oc}. Under these optimized conditions, the proposed device structure shows great potential as a high-efficiency, eco-friendly alternative to traditional thin-film technologies.

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