SCIENCE FORUM (JOURNAL OF PURE AND APPLIED SCIENCES) 26, (4) (2026), 150 - 158

Science Forum (Journal of Pure and Applied Sciences)

Journal Homepage: https://atbuscienceforum.com.ng/index.php/jpas
https://doi.org/10.70882/7efax756

Design and Performance Optimization of n-TiO_2/n-CdS/p-SnS heterojunction solar cell

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Abstract

Tin sulfide (SnS)-based photovoltaic devices have attracted considerable research interest as promising candidates for thin-film solar-cell applications because of their excellent semiconductor and optoelectronic properties. This study employed one-dimensional PC1D solar-cell simulation software to design and optimize an SnS-based heterojunction photovoltaic device and evaluate the influence of key absorber-layer parameters on device performance. The simulated solar-cell architecture consisted of three functional semiconductor layers: titanium dioxide (TiO_2) as the window layer, cadmium sulfide (CdS) as the buffer layer, and tin sulfide (SnS) as the photon-absorbing layer. The photovoltaic performance of the proposed TiO_2/CdS/SnS device was systematically investigated by varying the thickness and doping concentration of the SnS absorber layer. The principal photovoltaic parameters evaluated were the open-circuit voltage (Voc), short-circuit current density (Jsc), and power-conversion efficiency (η). The simulation results demonstrate that both absorber thickness and doping concentration exert significant effects on the photovoltaic characteristics and overall conversion efficiency of the device. Optimum performance was obtained at an SnS absorber-layer thickness of 2 μm and a doping concentration of 1.53×10^{17} cm^{-3}. Under these optimized conditions and at an operating temperature of 25°C, the simulated device achieved a maximum conversion efficiency of 14.87%, with a short-circuit current density (Jsc) of 20.93 mA/cm^2 and an open-circuit voltage (Voc) of 0.809 V. These findings demonstrate the potential of appropriately optimized TiO_2/CdS/SnS heterostructures for efficient thin-film photovoltaic applications and highlight the importance of absorber-layer engineering in improving SnS-based solar-cell performance.

Keywords
SnS material,
PC1D program,
Thin Films,
Solar Cells.
CdS Material.

ISSN 1119-4618
JPAS
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1. Introduction:

The latest challenge in the field of photovoltaics is the manufacturing of high-efficiency, low-cost solar cells in an environmentally friendly manner. For large-scale production, thin-film solar cells have demonstrated their ability to meet these expectations. Furthermore, thin-film technology enables the use of alternative materials, thereby overcoming the limitations of traditional silicon technology. To achieve an economic objective, researchers prioritized the use of materials that are abundant in nature, non-toxic, and inexpensive [1].

In recent years, tin monosulfide (SnS), a non-toxic material serving as an absorber layer has been considered a suitable alternative to silicon absorbers for the production of thin-film solar cells [2]. Its band gap is approximately 1.31 eV, which is close to the band gap value of silicon, However, the absorption coefficient is much higher reaching 10^5 cm^{-1}, this allows tin monosulfide to possess a better structure than the crystalline silicon layer [3]. A thin layer of tin sulfide (SnS) can absorb most photons in the solar spectrum with energies higher than the tin sulfide bandgap.

Furthermore, both tin and sulfur are materials available on Earth capable of providing vast amounts of solar energy daily. The use of these materials can also serve as an alternative to elements that are common yet scarce, such as cadmium, tellurite, gallium, and selenium [4]. In addition to the above, studies indicate the possibility of preparing tin sulfide (SnS) using low-cost methods such as spin coating, dip coating, and spray pyrolysis [5]. Consequently, eco-friendly solar cells featuring a tin sulfide absorption layer can be manufactured using a cost-effective technique. [4]. A theoretical study employing a ZnS/SnS structure with a buffer layer also indicates a theoretical efficiency of 12.08% [6]. When manufacturing SnS-based solar cells, it is also necessary to minimize optical losses including unwanted Fresnel surface reflection losses across the entire solar spectrum at the interface between the air and the cell's top layer in order to enhance light absorption. Better cell performance can be achieved by using materials with a wider bandgap, such as titanium oxide (TiO2), as a window layer, which facilitates the passage of photons to the SnS absorption layer.

2. Simulation of the SnS cell design and its configuration layout.

Researchers are working to increase the efficiency of thin-film solar cells through simulation using various available software programs, including COMSOL, SCAPS, AMPS, and PC1D. This study utilized the PC1d program, which is considered one of the most widely used commercially available solar cell modeling programs. Its success is attributed to its speed, ease of use, and continuous updates to incorporate the latest cell models. The PC1D software is now available for free from the University of New South Wales in Australia.

The raw source code for the PC1D program is also available to programmers and developers on the Source Forge platform. The program solves the fundamental equations for one-dimensional semiconductors namely, Poisson's equation and the electron and hole continuity equations which determine the electrical characteristics of the device under consideration [7, 8]. The PC1D program also yields simulation results that align well with experimental reports. Therefore, this program outperforms other solar cell simulation software.

An n-TiO2/n-CdS/p-SnS heterojunction solar cell has been designed, consisting of three layers: an n-type TiO2 window layer, a p-type SnS absorber layer, and an n-type CdS buffer layer situated between them, as illustrated in Fig. 1. Repeated attempts were made within the program to achieve the best performance for the solar cell, Repeated simulations were conducted to optimize the solar cell's performance by investigating the effects of the absorber layer's thickness ranging from (0.5 to 3)µm and doping concentration ranging from (10^{14} to 10^{20}) cm^{-3}. Additionally, the cell's output characteristics such as short-circuit current (Jsc), open-circuit voltage (Voc), and conversion efficiency (η) were determined using current-voltage (I-V) characteristic curves.

For each layer of the designed cell, fixed parameters such as the energy gap, dielectric constant, electrical permittivity, intrinsic charge carrier concentration, and others parameter were entered into the program. As for the remaining variable parameters, an initial sweep was performed using the "Batch" icon in the software to achieve the best solar cell performance. The operating temperature was varied between 25°C and 50°C to determine its effect on the cell's electrical characteristics. Additionally, the global AM 1.5 air mass spectrum and an irradiance of 100 mW/cm^2 were adopted for all simulations.

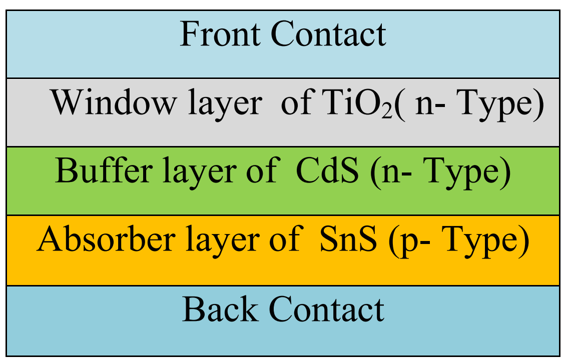

Figure (1). Shows the layers of the designed SnS cell.

Table (1) Simulation Parameters for the Designed Photovoltaic Cell.

Cell Elements	Its amount
Area of Cell	$1cm^2$
the depth of surface texture in forward	2 µm
the depth of surface texture in backward	2 µm
External reflectivity of the front face	8%
Front contact	Enabled
Rear contact	Enabled
Thickness of Window layer TiO2	0.08µm
Thickness of buffer layer CdS	0.1 µm
Thickness of absorber layer SnS	(0.5-3) µm

Back ground doping of Window layer	$6.87\times10^{16}cm^{-3}$
doping concentration of buffer layer	$1\times10^{18}cm^{-3}$
doping concentration of absorber layer	$(1\times10^{14}-1\times10^{20})cm^{-3}$
Forbidden energy gap of TiO2	3.35 eV
Band gap of CdS	2.42
Band gap of SnS	1.31
Dielectric constant of TiO2	9
Dielectric constant of CdS	10
Dielectric constant of SnS	13
Electron affinity of TiO2	4
Electron affinity of CdS	4.2
Electron affinity of SnS	4.1
Bulk recombination	$\tau_n = \tau_p$=1000μs
operating temperature	(25-50) °C
Incident light source	Air Mass 1.5g spectrum
Excitation Method	pulsed
External circuit of cell	extent from(-8 to 2)Volt

3. Results and Discussion

3.1 Effect of SnS absorption layer thickness

The effect of SnS absorption layer thickness on solar cell performance was evaluated by simulating the TiO2/CdS/SnS solar cell structure The thickness of the SnS layer was varied between 0.5 and 3 μm, while the thickness of the TiO_2 window layer was fixed at 0.08 μm and that of the CdS buffer layer at 0.1 μm .

Figure 2 illustrates the electrical characteristics specifically the current-voltage curves as the thickness of the SnS absorption layer varies; from these, the output characteristics of the photovoltaic cell (Voc, Jsc, and efficiency η) were determined. The results confirm that as the thickness of the SnS absorption layer increases, the current density (J) increases and becomes more stable across the voltage range.

This behavior indicates improved charge-carrier collection and reduced recombination losses compared to the thin layer. In other words, increasing the thickness of the absorption layer enhances light absorption, resulting in greater generation of electron-hole pairs [9]. It is observed in Figure (3) that as the thickness of the absorption layer increases to 2 μm, the short-circuit current Jsc increases from (11.5 to 23.88) mA/cm^2, and the open-circuit voltage Voc increases slightly from (0.803 V to 0.809) V,

This leads to an improvement in the cell's conversion efficiency, reaching 14.87%, as shown in Figure (3). As the thickness of the absorption layer decreases below 2 μm, the depletion region approaches the back contact, leading to an increased recombination rate. As a result, quantum efficiency decreases due to insufficient absorption of photons with long wavelengths, Consequently, both the open-circuit voltage (Voc) and the short-circuit current density (Jsc) will decrease. As the thickness increases to 2 μm, the tin sulfide (SnS) absorption layer generates more electron-hole pairs due to the absorption of more photons, thereby increasing the short-circuit current density and open-circuit voltage [10]. However, if the thickness of the absorption layer exceeds 2 μm, the electron-hole pair must travel longer distances, resulting in a slow rate of efficiency increase [10, 11] This reduction in cell efficiency may be attributed to several factors, including charge carrier recombination, as the minority carrier diffusion length in SnS is short.

This leads to increased series resistance resulting from the material's higher internal resistance and energy loss [12] . Therefore, the optimal value for the thickness of the SnS absorption layer is 2 μm. Figure (4) illustrates the variation of quantum efficiency (QE) with wavelength for each thickness value of the SnS absorption layer (0.5–3) μm. It has been observed that increasing the thickness of the absorption layer leads to higher quantum efficiency values; this signifies the absorption of a large number of photons from the electromagnetic spectrum incident on the cell and the generation of electron-hole pairs [13, 14].

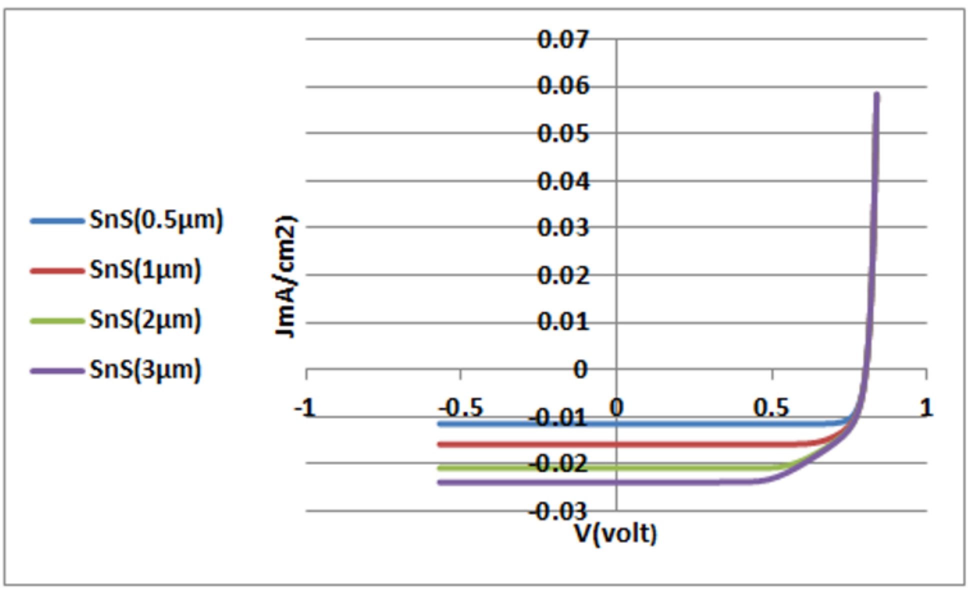

Figure (2). Current-voltage curve with varying SnS absorption layer thickness.

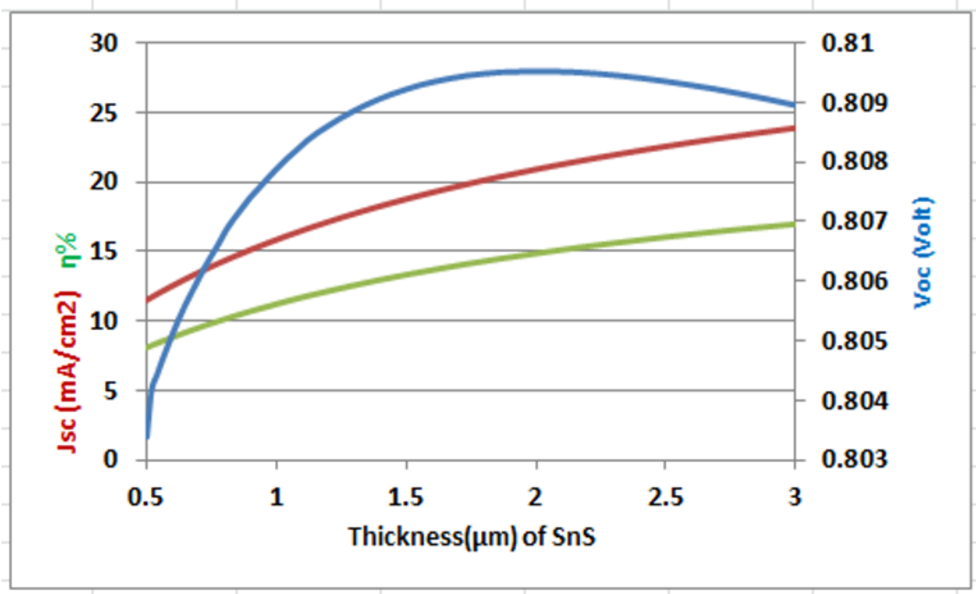

Figure (3). Variation of short-circuit current, open-circuit voltage and conversion efficiency with SnS absorption layer thickness.

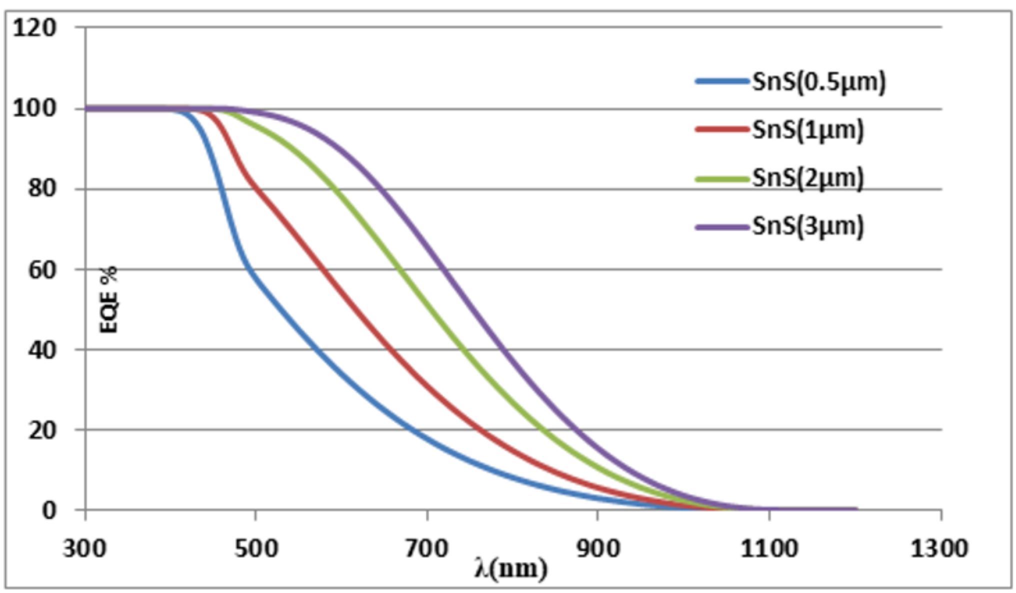

Figure (4). Quantum efficiency as a function of wavelength with varying SnS absorption layer thickness.

3.2 Effect of Doping Concentration on the SnS Absorption Layer

A crucial factor in solar cell design is the doping level; the effect of the doping concentration in the absorption layer ranging from (1×1014cm-3-1×1020cm-3) was investigated regarding the cell's output characteristics, specifically short-circuit current, open-circuit voltage, and conversion efficiency. It was observed that the open-circuit voltage (Voc) increased from (0.62 V-0.79V). With increasing the vaccination concentration from $1\times10^{14}cm^{-3}$ to $1.53\times10^{17}cm^{-3}$, then after this value a constant open-circuit voltage is achieved. The short-circuit current remains approximately constant at a value of 23.88mA/cm2 as the doping concentration increases up to 1.53 1017cm-3 beyond this value, the short-circuit current begins to decrease gradually with further increases in doping concentration. It was observed that increasing the doping level leads to higher Auger recombination losses. Therefore, the maximum doping concentration was set at 1×10^{20} cm^{-3}. By doping the absorption layer, impurities are introduced to create an electron deficiency or holes in the semiconductor material, which act as majority charge carriers. As the doping concentration increases, the number of available holes in the absorption layer rises, leading to improved charge carrier mobility. Based on our results, we observed that the short-circuit current density increases with increasing doping concentration. As the doping concentration increases from 1×10^{14} cm^{-3}. The internal electric field across the device also increases, which enhances the separation of photogenerated charge carriers and leads to an increase in open-circuit voltage and cell efficiency, as shown in Figure (5) [15].

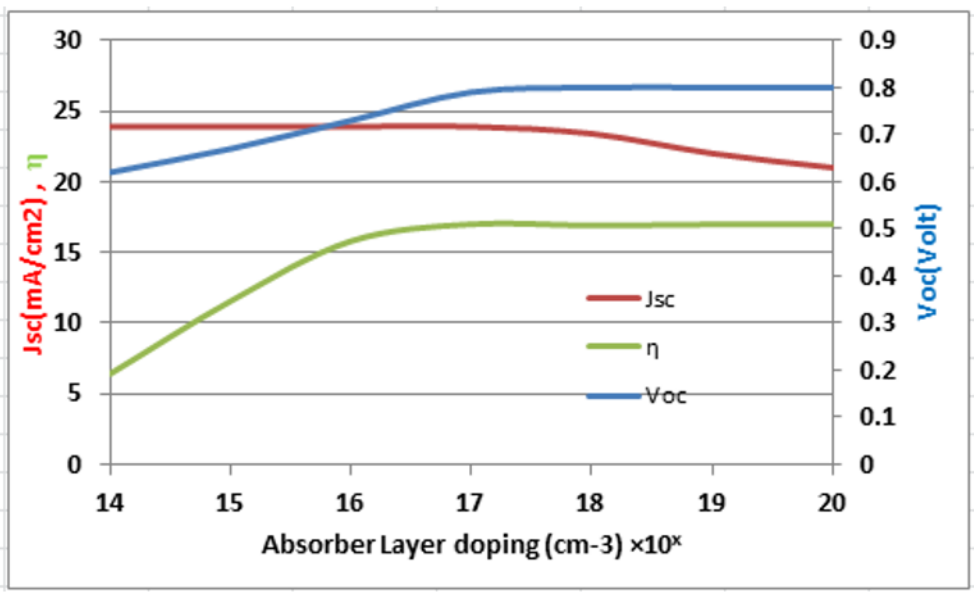

Figure (5). Variation of Voc , Jsc and η with the doping concentration of the absorption layer.

3.3 The effect of operating temperature on cell performance

The effect of temperature on tin sulfide (SnS) solar cells with different layers was investigated by varying the temperature from 25°C to 50°C. The thickness of the SnS absorption layer was fixed at 2 μm, while the thicknesses of the remaining layers were set to the optimal values discussed in the previous section for each structure. Table (2) illustrates the effect of temperature on solar cells made of tin sulfide with different layers. It has been observed that rising temperatures reduce the bond energy between electrons thereby increasing the speed of charge carriers and cause the energy gap of the semiconductor material to decrease. Consequently, the recombination rate of electrons and holes will increase, causing a slight decrease in the open-circuit voltage

[16]. However, Jsc increases slightly from 23.9mA/cm2 to 25mA/cm2 with increasing temperatures. Finally, conversion efficiency decreases slightly from 17% to 16.4% as the temperature rises, since conversion efficiency depends on Jsc and Voc.

Table (2) shows the effect of temperature on the output characteristics of the designed cell.

η %	Voc	Jsc	T °C
17	0.808	23.9	25
16.8	0.8	24.2	30
16.7	0.792	24.44	35
16.6	0.785	24.65	40
16.5	0.777	24.85	45
16.4	0.769	25	50

Conclusion

In this work, a numerical simulation of tin sulfide (SnS)-based solar cells was conducted using three different layers: titanium dioxide (TiO_2), cadmium sulfide (CdS), and tin sulfide (SnS). The electrical parameters were determined by varying the thickness and doping concentration of the absorption layer, in addition to studying the effect of temperature on the cell as a whole.

The main objective was to improve the absorption layer to achieve the best performance for the solar cell. The optimal electrical characteristics for the cell were achieved at an absorber layer thickness of 2 μm, yielding an efficiency of 14.87%, Jsc = 20.93 mA/cm^2, and Voc = 0.809 V. The optimal doping concentration for the absorption layer was 1.53×10^{17} cm^{-3}, and the optimal temperature was 25°C.

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