

Optimization of CIGS/CIGS Tandem Solar Cells by Adjusting Layer Thickness Using Silvaco-TCADe

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Highlights

- ❖ Design and simulation of CIGS/CIGS back-to-back solar cells using Silvaco-Atlas software
- ❖ Optimizing the performance of the CIGS/CIGS tandem solar cell
- ❖ Studying the effect of electrode metal and comparison of different materials

Graphical Abstract



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Optimization of CIGS/CIGS Tandem Solar Cells by Adjusting Layer Thickness Using Silvaco-TCAD

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ABSTRACT

This research designed and simulated CIGS/CIGS back-to-back solar cells using Silvaco-Atlas software. We considered CIGS absorbing layer thickness and sub-cells as critical parameters to optimize the performance of the CIGS/CIGS tandem solar cell. The research comparatively examined the effect of different electrode metals, such as molybdenum, aluminum, titanium, and silver, on the efficiency. The electrical parameters of the best CIGS/CIGS tandem solar cell configuration were a short-circuit current density (J_{sc}) of 15.65 mA/cm^2 , an open-circuit voltage (V_{oc}) of 1.86 V , a fill factor (FF) of 86.04% , and a conversion efficiency (η) of 27.12% . The optimal CIGS absorbing layer thickness of the top and bottom cells corresponding to the maximum conversion efficiency obtained were 0.17 and $6.3 \text{ }\mu\text{m}$, respectively. In contrast, the optimal thickness of the Cds layer was $0.04 \text{ }\mu\text{m}$. Silver had the best performance in connecting layers between several metals. The results can be used to develop low-cost and high-efficiency solar cells.

1. Introduction

Solar energy is a renewable energy that has the potential to produce energy for future generations. Every hour, Earth receives about four times as much solar energy as humans consume in a year. Therefore, if it can be converted into usable energy, such as electrical energy, we will no longer need to worry about the lack of energy in the world. In this regard, efforts in investigating and manufacturing solar cell devices have been growing in recent years [1]. Despite all the merits of thin-film cells compared to silicon cells, they suffer from the drawback of the amount of crystal defects, which increases electron-hole recombination in these cells. In thin-film solar cells, by calculating the appropriate thickness for the active layer versus the absorption coefficient, a process can be created to absorb all the wavelengths of light that shine on the cell. In the same vein, the propagation length of the electron-hole production created in the absorbent layer must be greater than the thickness of the absorbent layer in order to obtain a sufficient amount of electron-holes. Accordingly, choosing the suitable material with the proper thickness for thin-layer cells is very important. Amorphous silicon (a-Si), CIGS, and CdTe perform

best among various materials investigated in this field. These materials are used as absorbent layers in all thin-film cells due to their direct energy gap, high absorption coefficient, and compatibility of electrons with layers with higher energy gaps, such as CdS [2]. CIGS is one of the best candidates for making solar cells due to its unique properties, such as direct and controllable band gap energy, high radiation endurance, and the ability to deposit on flexible surfaces, such as metal foils [3]. The CIGS compound material has exceptional advantages, such as a high optical absorption coefficient (10^5 cm^{-1}) [4], a modifiable band gap from 1.02 eV for CuInSe₂ (CIS) up to 1.68 eV for CuGaSe₂ (CGS) [5], long-term stability, and high theoretical efficiency. High-efficiency CIGS-based devices can be made using many different manufacturing techniques [4]. The highest absorption coefficient in the CIGS layer is obtained when there is no gallium in the structure; that is, the layer acts as a CIS. Due to the high absorption coefficient of this layer, which is around 99%, the incoming photons are absorbed into this layer, and this absorption process occurs up to a depth of about one micron. This is why a thickness of one to two microns suffices when making a solar cell from this layer [6]. This becomes important if we need about three hundred microns of silicon to make a solar cell with silicon. The important thing is that although CuInSe₂ has a high absorption power, it has a small band gap energy. This problem can be solved by adding gallium. Some gallium atoms will replace indium, and the composition will be CuIn_xGa_{1-x}Se₂, which will achieve the highest efficiency by optimizing the amount of gallium to indium in this structure [7]. In today's world, the importance of solar cells has increased, so the goal is to make solar cells with higher efficiency and lower cost. Thin-film solar cells have a lower manufacturing cost than silicon solar cells, but their efficiency is lower. Therefore, this work aimed to optimize the performance of the double junction tandem solar cells based on CIGS/CIGS and extract the optimal electrical parameters of the structure studied. In this context, a numerical simulation of CIGS/CIGS tandem solar cell as a function of the CIGS absorbing layer thickness and its band gap of the sub-cells was performed using a two-dimensional device simulator Silvaco-Atlas in order to get the best structure simulated configuration, which corresponds the higher values of Voc for top and bottom cells and the good current matching between them.

2. Structure and simulation method

The CIGS/CIGS tandem solar cell structure considered in this study, which is schematically presented in Figure 1, consists of a double junction solar cell based on a CIGS connected optically and electrically with a ZnO layer as a transparent conducting oxide layer. The doping concentrations and thicknesses for different layers composing the structure simulated here are displayed in Figure 1. The detailed design of the CIGS top cell consists of a n-type ZnO transparent contact layer, a n-type CdS buffer layer, and a p-type CIGS absorbing layer. On the other hand, the bottom cell structure consists of a layer set composed of an n-ZnO window layer to ensure the electrical and optical connection between the two sub-cells, an n-CdS buffer layer, a p-CIGS absorbing layer, and finally, a

silver layer on a glass substrate usually used as the back contact. We used the TCAD Atlas simulator in Silvaco to simulate the solar cell. Atlas is a physically based two- and three-dimensional device simulator, which allows for solving Poisson's equation numerically coupled with the continuity equations for both electrons and holes under steady-state conditions. Physical models, such as Shockley-Reid-Hall (SRH) mechanisms, Auger and Langevin mechanisms of recombination, have been applied. In order to obtain the photon production rates along with the continuity equations, the solar spectra (AM1.5G) were imported into Atlas using the BEAM statement [8]. The change of current density versus voltage (J-V) under light was obtained, from which the main PV parameters were extracted, and J_{sc} , V_{oc} , fill factor (FF), and PCE were calculated. Then, the effect of the electrode metal and the thickness of the CIGS layers in the upper and lower cells were investigated and the most optimal state of the structure was obtained.

3. Simulation Results and Discussion

The CIGS/CIGS tandem solar cell structure obtained by Silvaco-Atlas is shown in Figure 2. The current density-voltage characteristics (J-V) of the CIGS/CIGS tandem cell are plotted in Figure 3 for the input base parameters given in Table 1.

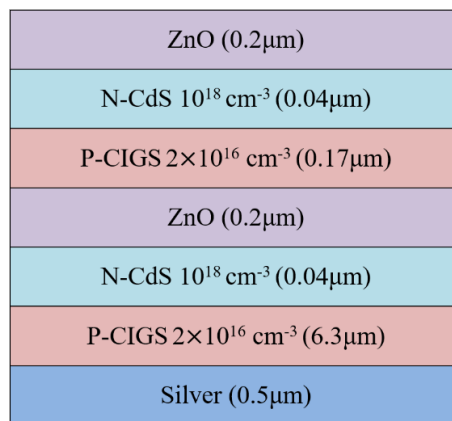


Figure1. The schematic structure of the CIGS/CIGS tandem solar cell.

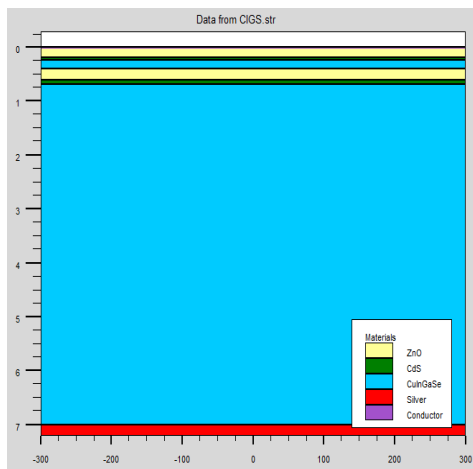


Figure 2. The Silvaco-Atlas structures file of the CIGS/CIGS tandem solar cell.

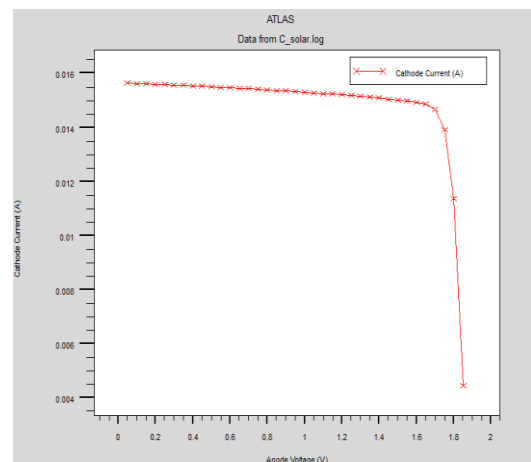
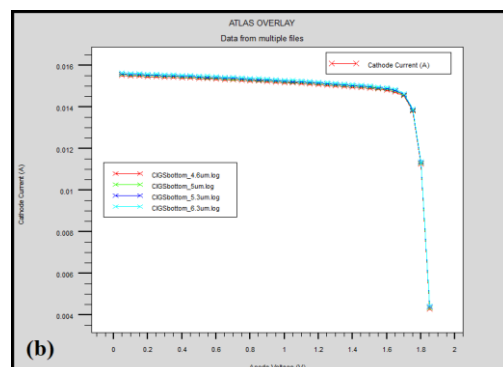
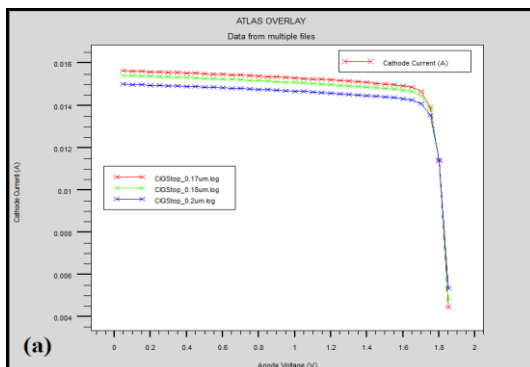


Figure3. The J-V characteristics of the CIGS/CIGS tandem cell before optimization.

Table 1. Material parameters used in the simulation.

Layer properties	ZnO	Cds	CIGS
E_g (eV)	3.3	2.4	1.13
ϵ_r	9	10	13.9
χ_e (eV)	4.1	4.5	4.8
μ_n (cm ² /Vs)	100	100	100
μ_p (cm ² /Vs)	25	25	25
N_c (cm ⁻³)	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}
N_v (cm ⁻³)	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}
Gaussian Defect States			
NDG, NVG (cm ⁻³)	D: 10^{17}	A: 10^{18}	D: 10^{14}
EA, ED (eV)	Mid gap	Mid gap	Mid gap
WG (eV)	0.1	0.1	0.1
σ_e (cm ²)	10^{-12}	10^{-17}	5×10^{-13}
σ_h (cm ²)	10^{-15}	10^{-12}	10^{-15}
Surface recombination velocity for electrons (holes) (cm.s ⁻¹)			
At CdS/CIGS interface	10^5	10^5	10^5
At CdS/CIGS interface	10^5	10^5	10^5
at front contact	10^5	10^5	10^5
at back contact	10^5	10^5	10^5

By matching the values of the short-circuit current density of the CIGS top cell and those of the bottom cell, we can determine the optimal CIGS absorbing layer thickness for the CIGS top cell, which corresponds to the good current matching between the sub-cells and leads to the maximum efficiency of the CIGS tandem cell. We varied the CIGS absorbing layer thickness of the CIGS top from 0.17 μm to 0.26 μm , and the thickness of the CIGS bottom cell from 5 μm to 6.3 μm . When the CIGS top cell is thicker, it absorbs more light, leaving less light to the CIGS bottom cell. Therefore, the CIGS bottom cell exhibits poor performance. For CIGS, the bottom cell's thicker layer means more light absorbance. Figure 4 indicates that J_{sc} increases by decreasing top CIGS and increasing bottom CIGS layer thickness. Figure 4(c) also illustrates that a thicker CdS buffer layer will allow more current to pass between the two cells. Using Silvaco software, we investigated the effect of the electrode and compared different materials, such as molybdenum, aluminum, titanium, and silver, on solar cell efficiency. As shown in Figure 5, silver metal performs best among the metals used in the solar cell structure under discussion. After that, aluminum, molybdenum, and finally, titanium are more suitable. According to the investigations in the previous sections, the optimal thickness for different layers was calculated, and the suitable metal for the electrodes was considered. Finally, electrical parameters J_{sc} , V_{oc} , FF, and η were calculated and compared with previous research. According to Table 2, we improved the structure.



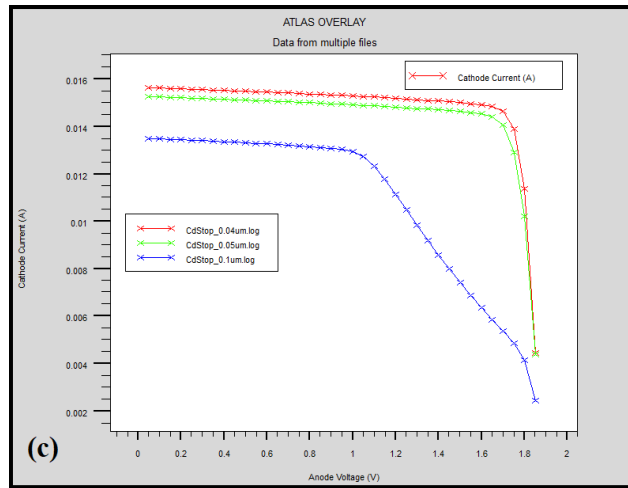


Figure 4. J-V characteristics of CIGS (a) top CIGS layer thickness, (b) bottom CIGS layer thickness, and (c) buffer layer thickness.

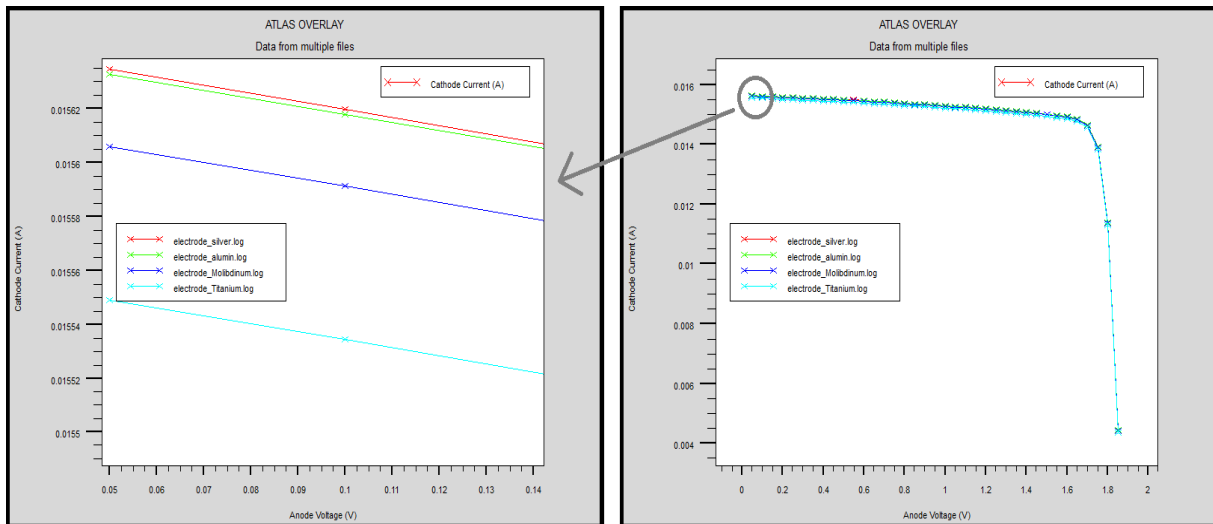


Figure 5. The J-V characteristics for different electrode metals.

Table 2. Electrical parameters of CIGS/CIGS tandem cell.

	J_{sc}	V_{oc}	FF%	$\eta\%$
Simulation [9]	16.35	1.80	85.09	25.11
Simulation [10]	16.89	1.77	82.54	27.03
Manufacture [11]	8.24	1.13	65.6	6.11
Our Simulation	15.65	1.86	86.04	27.12

4. Conclusions

CIGS/CIGS tandem cells with different thicknesses of CIGS absorber layers and different CdS for top and bottom cells were numerically simulated using Silvaco-Atlas to find the best CIGS/CIGS tandem solar cell configuration and select the optimal CIGS device parameters. After optimization, the conversion efficiency improved from 27.03% to 27.12% for a CIGS/CIGS tandem cell. The Voc value was equal to 1.86 V. It is equal to the sum of the separate voltages of the upper and lower cells. By matching the short-circuit current density values between the sub-cells ($J_{sc}=J_{sct}=J_{scb}$), we determined an excellent current match of 15.65 mA/cm² provided by the CIGS/CIGS tandem cell, increasing the performance of the simulated structure.

We considered the thickness of the CIGS absorber layer and CdS layer to improve the performance of the CGIS/CIGS tandem cell. It was found that the thickness of the optimal CIGS absorbing layer was 0.17 μm for the upper cell and 6.3 μm for the lower cell, and the thickness of the CdS layer was 0.04 μm. The most suitable metal for connecting was the silver electrode.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper. The ethical issues, including plagiarism, informed consent, misconduct, data fabrication and/or falsification, double publication and/or submission, redundancy, have been completely observed by the authors.

Credit Authorship Contribution Statement

Bahareh Boroomandnasab: Conceptualization, Formal analysis, Project administration, Supervision, Validation, Roles/Writing - original draft. **Mohammad Hossein Zolfaghari:** Conceptualization, Investigation, Methodology, Resources, Visualization, Writing - review & editing.

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