Global Journal of Engineering and Technology Advances

eISSN: 2582-5003

Cross Ref DOI: 10.30574/gjeta

Journal homepage: https://gjeta.com/

(Review Article)

Improvement of the Sb2Se3/Si tandem cell and simulation in SCAPS

Zuhair Dhnoon Mohammed * and Ayed Najem Saleh

Department of Physics, College of Education for Pure Sciences, Tikrit University, Iraq.

Global Journal of Engineering and Technology Advances, 2023, 17(03), 045–053

Publication history: Received on 09 November 2023; revised on 22 December 2023; accepted on 25 December 2023

Article DOI: https://doi.org/10.30574/gjeta.2023.17.3.0246

Abstract

In the work, tandem solar cells were designed to achieve improved efficiency using Sb2Se3/Si as the materials. The work involved simulating the Sb2Se3/Si structures, where Sb2Se3 served as the top cell and Si as the bottom cell, under AM1.5 G solar spectrum illumination using the one-dimensional device simulator Scaps. The obtained results demonstrated a significant increase in the efficiency of the Sb2Se3/Si tandem solar cell. Initially, the top cell had an efficiency of 14.29%, while the bottom cell had an efficiency of 11.22% when considered as single cells in a row. When used in tandem, the efficiency of the Sb2S3/Si tandem cell improved to 14.6%. Additionally, there were notable improvements in the electrical parameters of the solar cell. The overall efficiency (η) reached 21.41%, the open-circuit voltage (Voc) was 1.37volts, the short-circuit current density (Jsc) was 19.78 mA/cm^2, and the fill factor (FF) reached 78.62%. These results highlight the success of the Sb2S3/Si tandem solar cell in achieving higher efficiency and improved electrical performance compared to single cells.

Keywords: Solar cell; Tandem; Sb2Se3/Si; SCAPS-1D

1. Introduction

Energy production is indeed becoming an increasingly significant challenge for the future With the growth of industrial societies and the increasing global demand for energy the need for energy generation has become paramount [1]. In 2010 global demand was at (15 TW) and it is projected to require more than (30 TW) by the year 2050 [2]. It's important to note that this increased demand must be met without further carbon emissions ،as the associated environmental impact is a major concern. Currently ،a significant portion of the world's energy production comes from fossil sources, which are detrimental in terms of environmental pollution [3]. This has led to a growing interest in safe and renewable energy sources among scientists and technologists. Solar energy in particular, is considered a crucial component of renewable energy due to its cleanliness and potential to mitigate environmental impacts associated with conventional energy production.Solar power is recognized for its reliability the abundance of materials ،and ease of use. Solar cells specifically have gained widespread adoption and play a vital role in harnessing solar energy [4]. However single-junction solar cells have limitations due to their low energy conversion efficiency whereThe bandgap (Eg) of the absorber layer in these cells imposes restrictions on the absorption of light Photons with energy levels below the bandgap are not absorbed while those with energy levels above [5].To address these limitations tandem solar cells have been developed Tandem cells consist of two distinct cells: a top cell and a bottom cell. This approach leverages the concept of multi- junction solar cells, which have proven to be efficient [6]. Multi- junction solar cells feature different junctions with varying bandgaps (Eg) that are electrically interconnected through a thin layer. This configuration enables the absorption of a broader range of photons ،thereby enhancing overall energy conversion efficiency and reducing losses compared to single- junction cells Consequently ،tandem solar cells can absorb a larger portion of the solar spectrum with less energy loss ،especially in the long-wavelength spectra leading to higher efficiencies [7]. where the development of tandem solar cells is a promising solution to improve energy conversion efficiency and meet the growing global energy demands while reducing environmental impacts [8]. Solar energy remains at the forefront of

---

* Corresponding author: Zuhair D. Mohammed

renewable energy sources ،and advancements in tandem cell technology contribute to its continued growth as a clean and sustainable energy option. In the design of tandem solar cells, the optimization strategy focuses on ensuring that short-wavelength solar energies are primarily absorbed by the top subcell, while longer-wavelength solar energies pass through the top subcell and are preferentially absorbed by the bottom subcell. This design takes advantage of the differing bandgaps of the subcells to efficiently capture a broader spectrum of solar radiation [9]. By allowing photons to pass through the top subcell and be absorbed by the bottom subcell, tandem solar cells can achieve higher overall conversion efficiencies compared to single-junction cells. One effective approach to enhance light absorption in tandem solar cells is the insertion of interlayers between the top and bottom subcells. These interlayers play a crucial role by reflecting short-wavelength light back to the top subcell, increasing the chances of absorption and utilization of that energy. Simultaneously, the interlayers allow longer-wavelength light to transmit through to the bottom subcell, ensuring efficient absorption and utilization of that portion of the solar spectrum. The strategic management of light through interlayers contributes significantly to optimizing the overall performance and efficiency of tandem solar cells. In this particular study, a promising absorber material called Sb2Se3 was chosen due to its desirable properties. Sb2Se3 exhibits a high absorption coefficient, exceeding 10^4 cm, making it highly efficient in capturing sunlight. Additionally, it possesses a direct and optimal bandgap of approximately 1.6 eV, which aligns well with the solar spectrum. The monolithic tandem structure employed in this research consists of a bottom cell absorber layer made of silicon (Si), and a top cell absorber layer made of Sb2Se3. This configuration enables efficient utilization of the solar spectrum, with the Si bottom cell absorbing longer-wavelength light, while the Sb2S3 top cell absorbs shorter-wavelength light. By combining these materials in a tandem structure, the overall efficiency of the solar cell can be enhanced leading to improved performance in converting sunlight into electrical energy. Throughout the study, various aspects of the tandem solar cell were simulated and analyzed [10.11]. This involved exploring different parameters, such as the thickness of each subcell, the composition of interlayers, and the design of the device structure. Through these simulations, researchers were able to investigate the effects of these variations on the overall performance and efficiency of the tandem solar cell, contributing to the development of more efficient solar energy conversion technologies.

2. Methodology

Throughout this research endeavor, we employed the Solar Cell Capacitance Simulator (SCAPS-1D) software, specifically version 3.3.10 [12]. SCAPS-1D is a widely utilized computational tool expressly designed for the modeling and examination of solar cell performance. It ranks among the foremost programs in the realm of simulating and modeling thin-film polycrystalline solar cells. This software was originally conceived at Gents University within the Department of Electronics and Information Systems. Its functionality extends to facilitating the simulation of electrical properties, optical absorption, carrier transport, and various pertinent parameters of solar cell devices [13,14]. By harnessing SCAPS-1D, our research team conducted simulations and analyses of the tandem solar cell across a spectrum of conditions and variations .The software provides an extensive platform for probing the device's performance and fine-tuning its design parameters. SCAPS-1D has found widespread adoption in the photovoltaics field due to its precision in modeling and its contribution to the advancement and refinement of solar cell technologies. Numerical simulation is, indeed, an indispensable tool for scrutinizing and optimizing the performance attributes of Sb2Se3 solar cells. In this particular investigation, the upper cell structure is comprised of thin layers, encompassing ZnO, CdS, and Sb2Se3, representing the window, buffer, and absorber layers, respectively. Similarly, the lower cell incorporates ZnO, CdS, and Si layers, denoting the window, buffer, and absorber layers, in addition to rear contact layers. The model for the solar cell structure was implemented using the SCAPS simulation software, which facilitates the input of material and device parameters. Table 1 provides the essential material and device parameters required for the simulation. These parameters were derived from theoretical models, literature data, and, where experimental data was unavailable, estimated values were employed [15, 16]. Through the utilization of numerical simulation with SCAPS, our research team effectively assessed the performance characteristics of Sb2Se3 solar cells under diverse conditions. This enabled the optimization of the device's structure and an evaluation of the impact of various parameters on its overall efficiency. This approach aids in guiding experimental optimization and furnishes valuable insights into the behavior of solar cells, ultimately enhancing their performance and dependability.

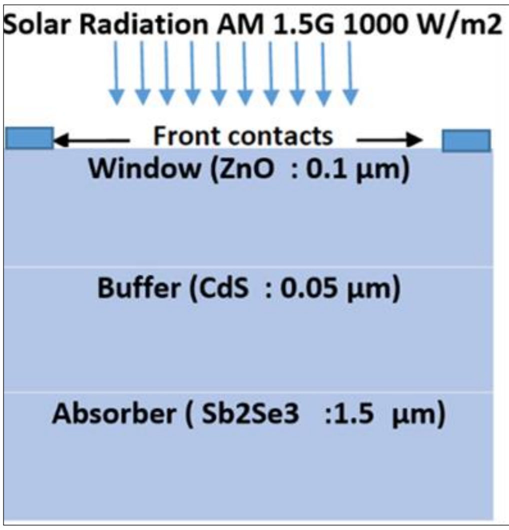

Figure 1 A Schematic of single Sb2Se3 top cell

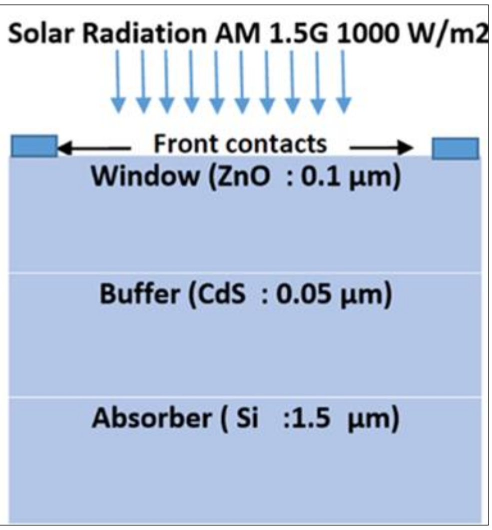

Figure 1 B Schematic of single Si bottom cell

Figure 1A illustrates single-designed solar cells. The figure clearly depicts the presence of a (ZnO) window layer and a (CdS) buffer layer, with an underlying (Si) absorption layer. Similarly, Figure 1B represents a standalone solar cell, specifically a top cell comprising a (ZnO) window layer, a (CdS) buffer layer, and an (Sb2Se3) absorption layer.Initially, we conducted an investigation into the structures of single-junction solar cells, namely (Sb2Se3) and (Si), individually. This examination aimed to discern the differences in efficiency and thickness and their impact on cell performance when comparing single cells to tandem cells.The top and bottom subcells are intricately interconnected as depicted in Figure 1C showcasing the (Sb2Se3/Si) tandem solar cell's.

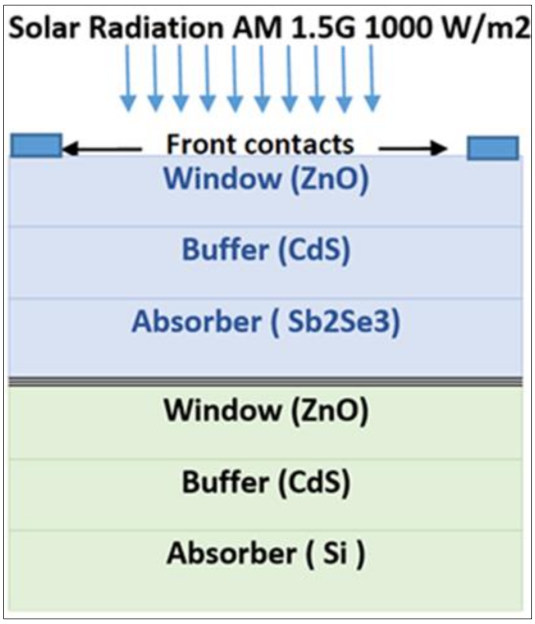

Figure 1C Structure of Si/Sb2Se3 tandem solar cell

Table 1 Basic material parameters used in the simulation

Parameter and units	**Sb2Se3**	**Si**	**CdS**	**ZnO**
Thickness (um)	1.5	1.5	0.05	0.1
Band gap (eV)	1.5	1.12	2.4	3.3
Electron affinity (eV)	4.04	4.05	4.2	4.6
Dielectric permittivity ε,	18.000	11.9	10	9
Effective conduction band density (cm-3)	2.2E+18	2.8E19	1.8E19	2.2E18
Effective valence band density (cm-3)	1.8E+19	1.04E19	2.4E19	1.8E19
Electron thermal velocity (cm/s)	1E7	1E7	1E7	1E7
Hole thermal velocity (cm/s)	1E7	1E7	1E7	1E7
Electron mobility (cm2 V-1 s -1)	15	1.5E3	100	100
Hole mobility (cm 2 V-1 s -1)	5.1	4.5E2	25	25
Doping concentration of donors (cm -3)	0	1E10	1E17	1E18
Doping concentration of acceptors (cm-3)	1E13	1E10	10	1E5

3. Results and Discussion

The results presented in this section are systematically arranged. The simulations of single cells as well as the top and bottom cells of the tandem structure have been conducted in an orderly fashion. Then we have also modeled and simulated the homogenous tandem structure encompassing the combination of the top and bottom layers.

3.1. Modeling and simulation of single top and bottom Sb2Se3/ Si solar cells

Within this section, we conducted simulations of the structures of single-junction solar cells, specifically Sb2Se3 and Si. These simulations were performed using the physical parameters and constants outlined in Table 1. A thickness of 1.5 um was selected as it was determined to be the optimal thickness for the cell in terms of current and efficiency. current and voltage is shown in Fig 2 for both the top and bottom cells The simulation of the device top single cell gave an efficiency (η) of 14.29 %, short circuit current (J) of 26.43 mA/cm^2 , an open circuit voltage (V) of 0.83 V and the fill factor (FF) of 65.16 % . As for the bottom single cell gave an efficiency (η) of 11.22 %, short circuit current (J) of 42.13 mA/cm^2, an open circuit voltage (V) of 0.38 V and the fill factor (FF) of 69.3%

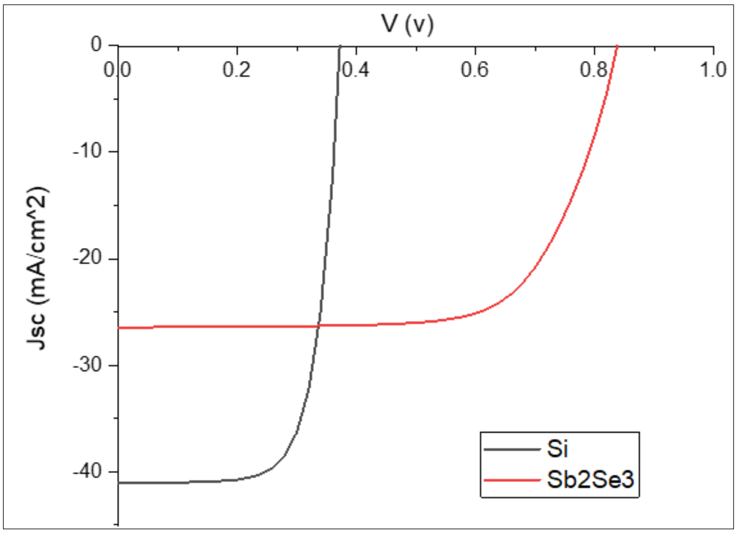

Figure 2 I- V plot of model of top and bottom solar cell

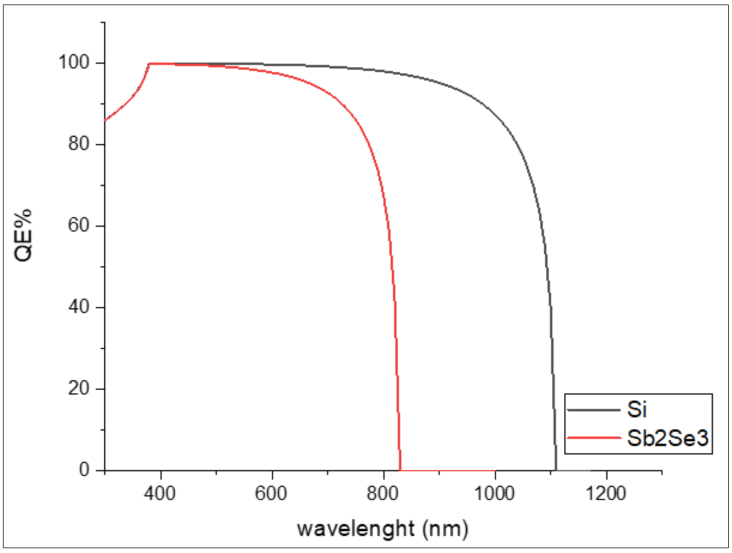

Figure 3 The variation of QE with wavelength (λ) for the Sb2Se3 / Si

Figure 3 portrays the quantum efficiency (QE) curves for individual solar cell components. Quantum efficiency (QE) is a measure of the ratio between the output charge carriers (electron-hole pairs) and the incident photons. The plot illustrates how QE varies for the fundamental Sb2Se3 and Si solar cells in relation to the absorption layer, which in this context includes Sb2Se3 and Si. The graph delineates the portion of the incident wavelength range that efficiently transforms light into electron-hole pairs, subsequently collecting them as electrical current within the solar cell. This visual representation offers valuable insights into the efficiency of the cell in converting different wavelengths of light into electrical current By scrutinizing these quantum efficiency curves, researchers can assess the cell's performance across varying wavelengths and pinpoint areas where conversion efficiency is either high or low. Such analysis is pivotal for comprehending the spectral response and overall efficiency of the solar cell, thereby contributing to the optimization and design of the cell to enhance its performance across the entire solar spectrum [17].

3.2. Design and analysis of Sb2Se3/Si tandem solar cell structure

Figure 1C provides a schematic representation of the Sb2Se3/Si tandem solar cell structure, illustrating a double-junction, monolithic tandem solar cell with a series connection between the cells. The arrangement of these cells is determined by their respective energy bandgaps, with the upper cell having a larger bandgap and the lower cell featuring a smaller bandgap. This strategic design ensures that the tandem structure can efficiently capture a broader spectrum of solar radiation, thereby maximizing the current output [18].The proposed top cell is composed of an Sb2Se3 absorber layer with a bandgap of 1.5 eV, while the bottom cell incorporates a Si absorber layer with a bandgap of 1.1 eV [10, 19]. The selection of these specific bandgaps allows for effective absorption of the maximum available solar flux. In Figure 4 the current density variation is depicted for both the top and bottom cells. Notably, the short-circuit current density (Jsc) of the top cell increases as the thickness of the top subcell increases, which can be attributed to the heightened incident solar power. To achieve current matching between the top and bottom cells (matching Jsc), it is imperative to strike a balance between the thicknesses of the two subcells. As the thickness of the top subcell increases, the Jsc (short-circuit current density) of the top cell tends to rise, while the Jsc of the bottom cell decreases. This phenomenon can be elucidated by considering the absorption properties of the top and bottom subcells. When the top subcell is exposed to sunlight, it absorbs a larger portion of the incident light, resulting in a higher current output (Jsc) for the top cell. However, due to the increased absorption by the top subcell, less light is transmitted through to the bottom subcell, leading to a reduction in the Jsc of the bottom cell. This phenomenon arises because the thick top cell absorbs a significant amount of light, thereby diminishing the amount of light that reaches the bottom cell. Consequently, in this scenario, achieving current matching can be realized by increasing the thickness of the Sb2Se3 layer while maintaining a constant thickness for the Si layer.

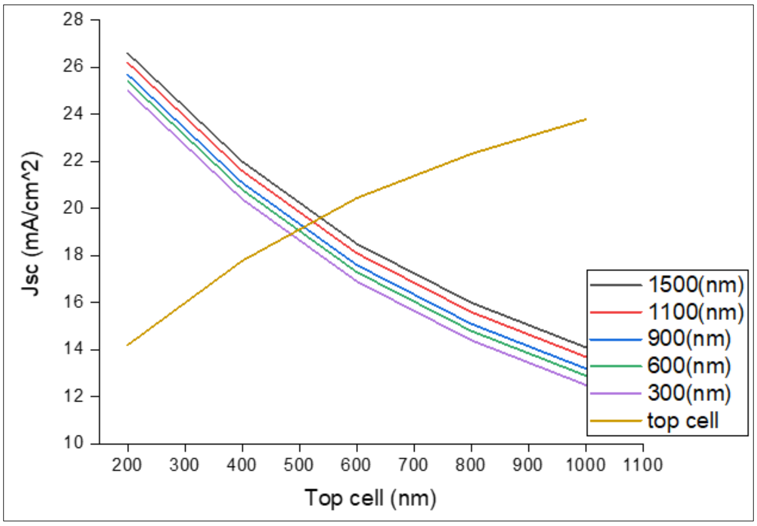

Figure 4A Matched current of the top cell (Sb2Se3) and bottom cell (Si) Electrical

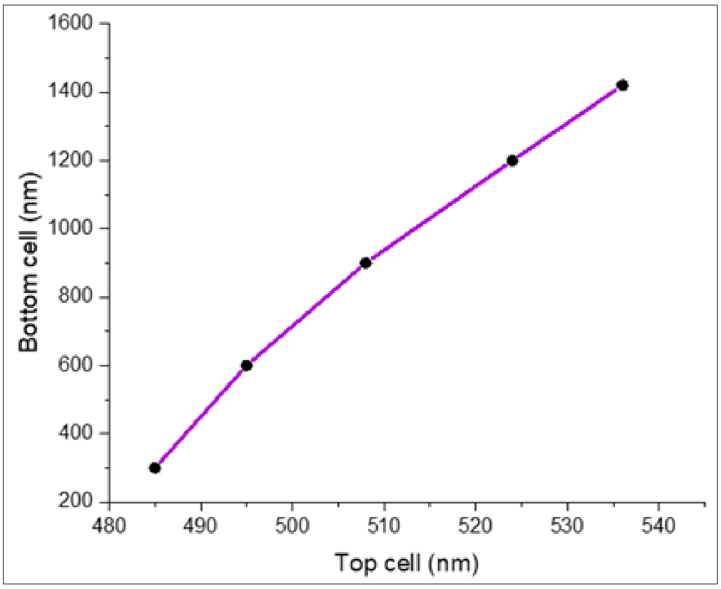

Figure 4 B The thickness of the upper and lower cell when matching the current

Table 2 Electrical characteristics of the top cell and the bottom cell when matching current

Thickness Bottom cell (nm)	**Top cell thickness (nm)**	**Carrent matching Jsc mA/cm²**	**Voc top cell volt**	**FF top cell %**	**Efftop cell %**	**Voc bottom cell volt**	**FF bottom cell %**	**Eff bottom Cell %**
300	485	18.85	0.8231	71.19	11.04	0.4944	74.46	6.93
600	501	19.14	0.8257	71.43	11.28	0.4972	74.68	7.10
900	512	19.35	0.8284	71.68	11.48	0.502	74.93	7.27
1100	523	19.52	0.8326	71.97	11.69	0.522	75.12	7.65
1500	536	19.78	0.8343	72.13	11.9	0.543	75.37	8.09

Table 3 Electrical properties of tandem cell (Sb2Se3)

Thickness Bottom cell (nm)	Top. cell thickness(nm)	Jsc mA/cm2	V(volt)	FF %	Eff %
300	485	18.85	1.3175	77.66	19.28
600	501	19.14	1.3229	77.98	19.74
900	512	19.35	1.3304	78.25	20.14
1100	523	19.52	1.3546	78.43	20.73
1500	536	19.78	1.3773	78.62	21.41

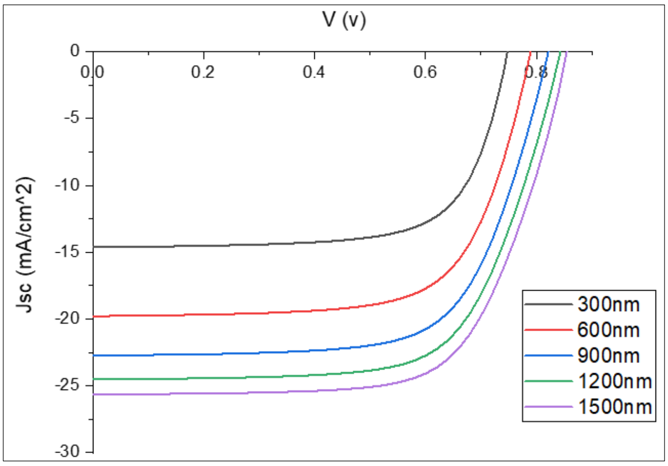

Figure 5 (I – V) of tandem solar cell

It was determined that the most efficient tandem cell, with thicknesses of 1500 nanometers for the top cell and 536 nanometers for the bottom cell, achieved an impressive cell efficiency of approximately 21.41%. This outstanding efficiency is highlighted in Table 3 and visually depicted in Figure 5 where the current-voltage (I-V) characteristics of the tandem cell, comprising the Sb2Se3 top cell and the Si bottom cell, are presented. These I-V curves serve as valuable tools for gaining insights into the current (J) and voltage (V) characteristics of the tandem cell. The short-circuit current density (Jsc) curve, for instance, portrays the cell's current output at zero applied voltage, illustrating the maximum current generated when there is no resistance in the circuit. Conversely, the open-circuit voltage (Voc) curve showcases the voltage output of the tandem cell in the absence of any current flow, signifying the maximum voltage obtainable from the cell under open-circuit conditions. These I-V curves collectively offer a comprehensive view of the cell's performance [20].

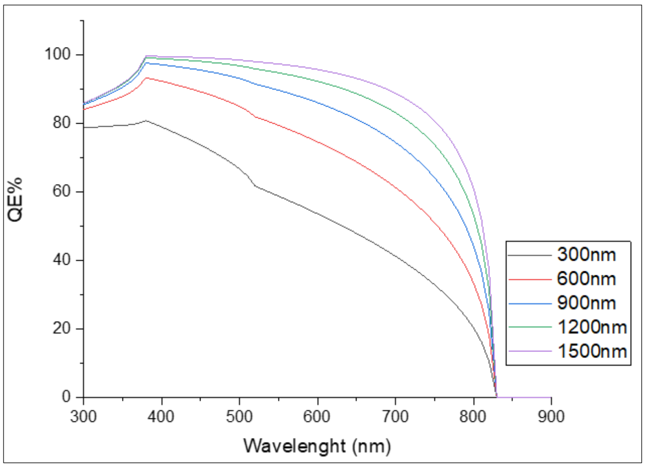

Figure 6 The variation of QE with wavelength (λ) for the tandem solar cell

In Figure 6, it is evident that the quantum efficiency of the tandem cell surpasses that of the single cells, signifying an enhanced ability to convert light into electrical energy across a wide spectrum of wavelengths. Notably, the performance of the Sb2Se3/Si tandem solar cell excels in comparison to the Sb2Se3 single solar cell. This improvement is attributed to the tandem cell's ingenious design, which capitalizes on the differing bandgaps of its top and bottom cells to enhance the absorption of photon energy over a broad range of wavelengths. The top cell, characterized by a higher bandgap, is optimized for absorbing longer wavelengths of light, while the bottom cell, featuring a lower bandgap, is better suited for capturing shorter wavelengths. This strategic configuration allows for the generation of photocurrent across a wide spectral range, ultimately leading to superior overall efficiency for the.

Through rigorous device simulations, the tandem solar cell achieved impressive metrics: an efficiency (η) of 21.41%, a short-circuit current (J) of 19.78 mA/cm2, an open-circuit voltage (V) of 1.37 V, and a fill factor (FF) of 78.62%. These quantifiable parameters offer a precise measure of the tandem cell's performance and underscore its superior efficiency when compared to individual single cells. These results underscore the substantial potential of the Sb2Se3/Si tandem solar cell in attaining heightened efficiency and more effective utilization of the solar spectrum for enhanced energy conversion. Such findings are instrumental in the optimization and design of future tandem solar cell structures aimed at even greater efficiency and improved energy conversion capabilities.

4. Conclusion

In our research endeavor we undertook numerical modeling and simulation of Sb2Se3/Si structures utilizing the Solar Cell Capacitance Simulator (SCAPS-1D). Our primary objective revolved around elevating the efficiency of a novel tandem configuration based on Sb2Se3/Si materials. Our work encompassed extensive numerical simulations to evaluate the performance of both single-junction Sb2Se3 and Si solar cells, in addition to a dual-junction Sb2Se3/Si tandem solar cell, all operating under the AM1.5 G light spectrum .Through these simulations, we elucidated the J-V (current-voltage) characteristics and essential photovoltaic(PV) parameters Initially we optimized the single-junction Sb2Se3 and Si solar cells individually achieving conversion efficiencies of approximately 14.29% and 11.22%, respectively. Subsequently, we delved into the performance analysis of a dual-junction Sb2S3/Si tandem solar cell configuration, featuring Sb2Se3 as the top cell and Si as the bottom cell. Impressively ths endeavor yielded a significant enhancement in conversion efficiency culminating in a remarkable 21.41% efficiency for the Sb2S3/Si tandem structure. This improvement was made possible through judiciously chosen thicknesses for both the top and bottom cells.

Our research underscored the advantages of a series connection between the top and bottom cells, resulting in mitigated limitations in short-circuit current and the overlay of open-circuit voltage characteristics. In summation, our study contributes substantively to the progression of tandem solar cell designs based on Sb2S3/Si. Through rigorous numerical simulations, we have acquired crucial insights into the performance characteristics of single-junction and tandem solar cells, providing invaluable information for the optimization and advancement of efficient photovoltaic devices.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

References

[1] International Energy Outlook, U.S. Energy Information Administration, 2011.

[2] S. Sinha, D. K. Nandi, S. Kim, and J. Heo. Atomic-layer-deposited buffer layers for thin film solar cells using earth-abundant absorber materials : A review. Solar Energy Materials and Solar Cells 2018; 176: 49–68

[3] Kleijn, R., van der Voet, et al, Metal requirements of low-carbon power generation, Energy 36, and 5640–5648, 2011.

[4] Vesborg, P.C.K., Jaramillo, Addressing the terawatt challenge: scalability in the supply of chemical elements for renewable energy. RSC Adv. 2, 7933, 2012.

[5] A. Bhuiyan, K. Sugita, A. Hashimoto, A. Yamamoto, InGaN solar cells: present state of the art and important challenges, IEEE J. Photovoltaic. 2276–293, 2012.

[6] L. Hsu, W. Walukiewicz, Modeling of InGaN/Si tandem solar cells, J. Appl. Phys. 104, 024507, 2008.

[7] R. Santbergen, H. Uzu, K. Yamamoto, M.J.I.J.o.P. Zeman, ptimization of Three- Terminal Perovskite/Silicon Tandem Solar cells, 9 , 446–451, 2019.

[8] K. Kim, J. Gwak, S.K. Ahn, Y.J. Eo, J.H. Park, J.S. Cho, M.G. Kang, H.E. Song, J.H. Yun, Simulations of chalcopyrite/c-Si tandem cells using SCAPS-1D, Sol Energy, 145, 52–58, 2017.

[9] Nicole Doumit,* Kahatie Soro, Aylin Ozocak, Nathalie Batut, Ambroise Schellmanns, Eddy Saintaime, and Esidor Ntsoenzok,Boosting the Efficiency of CZTS/Si Tandem Solar Cells Using In2O3 Layer in CZTS Top Cell, Adv. Theory Simul, 4, 2100099, 2021.

[10] Abdul Kuddus, Abu Bakar Ismail, Jaker Hossain, Design of a highly efficient CdTe-based dual-heterojunction solar cell with 44% predicted efficiency, Solar Energy 221 , 488–501, 2021.

[11] Mohamed Bouaouina, Contribution to the study and optimization of the performance of solar cells based on GaAs and Si, Master's thesis in energy physics. University of Constantine, 2001.

[12] Burgelman, M., Decock, K., Niemegeers, A., Verschraegen, J., & Degrave, S, SCAPS manual, 2021.

[13] M. Burgelman, P. Nollet, S. Degrave, Modeling polycrystalline semiconductor solar cells, Thin Solid Films 361–362 ,527–532, 2000.

[14] S. Degrave, M. Burgelman, P. Nollet, Modelling of polycrystalline thin film solar cells: new features in SCAPS version 2.3, in: Proceedings of the 3rd World Conference on Photovoltaic Energy Conversion, WCPEC-3, Osaka, pp. 487–490, 2003.

[15] Arindam Basak, Udai P. Singh , Numerical modelling and analysis of earth abundant Sb2S3 and Sb2Se3 based solar cells using SCAPS-1D , Solar Energy Materials & Solar Cells, 230 , 111184, 2021.

[16] Zhen-Qi Li, Ming Ni and Xiao-Dong Feng, Simulation of the Sb2Se3 solar cell with a hole transport layer, Mater. Res. Express 7, 016416, 2020.

[17] Adeyinka D. Adewoyin, Muteeu A. Olopade, Olusola O. Oyebola, Micheal A. Chendo, Development of CZTGS/CZTS tandem thin film solar cell using SCAPS-1D, Optik, 2019

[18] M. Elbar, S. Tobbeche, A. Merazga ,Effect of top-cell CGS thickness on the performance of CGS/CIGS tandem solar cell, Solar Energy (2015) 122 , 104–112

[19] Saugata Sarker, Md Tohidul Islam, A SCAPS simulation investigation of non-toxic MAGeI3-on-Si tandem solar device utilizing monolithically integrated (2-T) and mechanically stacked (4-T) configurations,Solar Energy 225, 471–485, 2021.

[20] Fatima Rehman,Iqrar Hussain Syed, et al,Fourth-generation solar cells: a review, Cite this: Energy Adv, 2, 1239, 2023.