Improvement of CISSe / CdS / ZnO Structure Performance by SCAPS-1D.

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Abstract

This manuscript presents an optimization of the performances of the CISSe/CdS/ZnO structure. 12 tests were performed for each layer on thickness, gap energy and temperature using SCAPC-1D. Numerical data were compiled with the open circuit voltage, the short circuit density, the fill factor and the efficiency. The results obtained are confirmed with the measurements illustrated in the literature. The analyses indicate a progressive improvement in the performance of the structure for each test; an efficiency of 28.8 % was recorded for the CISSe layer while 30.07 % as an efficiency for CdS and 31.47 % for the absorbent layer. On the other hand, an open circuit voltage does not exceed 1.37V for the whole structure. Thus, these results are satisfied and encouraged.

Highlights:

Optimization of the performance of the CISSe/CdS/ZnO layer.

Performing 12 tests on the four characteristics of each layer.

Achievement of 30.47 % efficiency for the main layer in the cell.

Introduction

The development of high efficiency and low cost solar cells is one of the challenges for most manufacturers in this field. Therefore, research has accelerated to find a structure which has high energy production capacities and which depends on non-toxic materials. Semiconductors are considered to be one of the efficient and innovative solutions. These thin films have many properties such as the ability to adjust its bandgap, thickness and even the doping method. One of the most famous of semiconductors are CISSe, CdS and ZnO. These three layers have been used in the construction of many structures with great capacities, high efficiency and very encouraging cost. Copper indium sulfoselenide, $\text{CuIn}(\text{S}, \text{Se})_2$ is an inorganic nanocrystalline chalcogenide, Its efficiency varies between 18.08 % and 22.50 % [1], [2] depending on the role it plays in the structure. On the other hand, CdS cadmium has a bad reputation which is harmful to the environment, but recently discovered treatment methods have reduced its toxicity [3]. The ZnO layer is a main element in the fabrication of structures of photovoltaic systems, which shows an efficiency can reach up to 17.86 % [4] - [6]. Therefore, configuring a structure based on these perovskite cells will be a huge boost to the solar cell industry.

In this article, the CISSe/CdS/ZnO structure is highlighted in order to develop its performance and evaluate its efficiency. This structure where CISSe is a window layer, CdS is a conductive layer and ZnO is absorbent. A set of tests will be carried out on the thickness, the gap energy and the temperature for each layer under the effect of a radiation of 1000w/m^2 (see figure 1). By using the SCAPS-1D software, some analyses are carried out on current density, fill factor and voltage.

Methodology

The methodology is based on performing three basic tests related to each layer. In the first step, the thickness, the gap energy (E_g) and the temperature are tested in the intervals [0.1 eV; 2 eV], [1 μ m; 50 μ m] and [300K, 350K] respectively for the CISSe layer. Data will be compiled on these fourth characteristics including Voc, Jsc, FF and efficiency(η). For an easy evaluation, these characteristics will be named according to the layer that contributed to modification. During all tests, table.1 is approved in the evaluation process. The second and third stages will be carried out following the same procedure to study the CdS and ZnO layers through different intervals which will be indicated in the continuation of this research. It should be noted that there are 9 tests carried out on the CISSe/CdS/ZnO structure.

Tab.1.Physical property of the layers used.

Physical property	Symbols	Window layer CISSe	Buffer layer CdS	Absorber layer ZnO
Electron affinity (eV)	χ	4.300	4.100	4.100
Dielectric permittivity (relative)	ϵ_r	4.300	9.000	9.000
CB effective density of states (1/cm ³)	N_c	12.000	3.00×10^{18}	4.00×10^{18}
VB effective density of states (1/cm ³)	N_v	1.000×10^{19}	1.800×10^{19}	1.00×10^{19}
Electron thermal velocity (cm/s)	V_e	1.000×10^{19}	1.00×10^7	1.00×10^8
Hole thermal velocity (cm/s)	V_h	1.00×10^7	1.00×10^7	1.00×10^8
Electron mobility (cm ² /Vs)	μ_p	1.000×10^7	1.00×10^2	1.00×10^2
Hole mobility (cm ² /Vs)	μ_n	1.000×10^7	2.500×10^2	2.500×10^1
Shallow uniform donor density (1/cm ³)	N_A	1.000×10^5	1.00×10^5	1.00×10^{18}
Shallow uniform acceptor density (1/cm ³)	N_D	1.000×10^{16}	1.00×10^5	1.00×10^5

Simulations And Results

CISSe layer optimization

The $E_{g,CISSe}$ will be varied from 0.1 eV to 2 eV with a step of 1 eV. Fig.2 illustrates the results obtained for the four parameters $J_{sc,CISSe}$, $V_{oc,CISSe}$, EF_{CISSe} , h_{CISSe} .

Fig.2-a ,shows the stability of the J-V characteristics between 0.1 eV and 1.0 eV for the values; $J_{sc,CISSe} = 43,57$ mA/cm²; $V_{oc,CISSe} = 0,843$ V. After that, we noticed a sudden decreasing change of these two characteristics, then increase in their values until reaching the maximum $J_{sc,CISSe}(max) = 43,58$ mA/cm²; $V_{oc,CISSe}(min) = 0,7597$ V, with $E_{g,CISSe} = 1.7$ eV. After the characteristics know a stability in their values. In Fig.2-b we also held the same comment for the couple (EF_{CISSe} , h_{CISSe}) where the stability was

recorded in the same period for the pair, and after that, a maximum increase has been known at the point $E_{g,CISSe} = 1.7$ eV where a higher efficiency was obtained $h_{CISSe} = 27.56$ % and $EF_{CISSe} = 83.26$ %. This value found will be analysed according to the thickness of the window layer.

Fig.3-a shows the evolution of the current density and the voltage as a function of the width of the Window layer. The thickness will be varied between $1\mu m$ and $50\mu m$ with a step of 1 and the E_g set in 1.7 eV of CISSe. We notice a significant increase in the couple J_{sc} , V_{oc} from the start of the thickness until to the value $15\mu m$. From this value, we notice the inflection of the two curves, but with a slight continuation of their rise until they reach maximum values $J_{sc,CISSe}(\max) = 45.35 mA/cm^2$, $V_{oc,CISSe}(\max) = 0.843$ V at $20\mu m$ thickness. The results of Fig.3-b indicate a significant increase in efficiency η (%) up to the maximum value $\eta_{CISSe}(\max) = 30.07$ % for the same thickness. On the other hand, an accelerated decrease in EF_{CISSe} as a function of thickness. Therefore, the efficiency was improved and linked to the thickness. Finally, we can say that at $20\mu m$ with $E_{g,CISSe} = 1.7$ eV, we obtain an ideal efficiency of the CISSe window layer compared to the measurements indicated in [7], [8].

For the thickness $20\mu m$ and $E_{g,CISSe} = 1.7$ eV, Fig.4-a and Fig.4-b show the variation of the characteristics of the two pairs ($J_{sc,CISSe}$; $V_{oc,CISSe}$) and (EF_{CISSe} ; h_{CISSe}). Between 300K and 350K, the temperature enhances the mobility of electrons in the Se window layer; result well explained by Fig.3-a by the increase of J_{sc} . On the other hand, the parameters $V_{oc,CISSe}$; EF_{CISSe} ; h_{CISSe} decrease to minimum values $V_{oc,CISSe}(\min) = 0.843$ V; $EF_{CISSe} = 75.87$ %; $h_{CISSe}(\min) = 28.8$ %, result considered positively by comparing with the results recorded in [9], [10].

CdS layer optimization on $20\mu m$ CISSe thickness and $E_{g,CISSe} = 1.7$ eV

The second test will be carried out on the study of the buffer of the CdS layer at a temperature of 300K under the following conditions. $E_{g,CISSe} = 1.7$ eV, $E_{g,ZnO} = 3.3$ eV. The thicknesses of CISSe and ZnO will be fixed at $20\mu m$ and $0.2\mu m$. $E_{g,CdS}$ will be varied between 0.1 eV and 3.5 eV with a step of 0.5 eV. The results obtained are shown in Fig.5.

Fig.5-a illustrates the variation of $J_{sc,CdS}$ and $V_{oc,CdS}$ under the effect of the $E_{g,CdS}$. We notice between 0.1 eV and 1.0 eV, there is an overlap between the two curves at the level of their variation. After the value of 1 eV, the two parameters increase to a maximum value $J_{sc,CdS}(\max) = 45.35 mA/cm^2$, $V_{oc,CdS}(\max) = 0.8436$ V when the value of $E_{g,CdS} > 2$ eV. As for Fig.5-b, it shows a quasi-agreement between the curve EF_{CdS} and η_{CdS} at the level of their evolutions until they reach the constant values indicating a maximum efficiency $\eta_{CdS} = 30.06$ % and $EF_{CdS} = 78.87$ % when the energy $E_{g,CdS} > 2$ eV.

The curves of $J_{sc,CdS}$, $V_{oc,CdS}$ illustrated in Fig.6-a make it possible to show the effect of CdS layer thickness while setting the $E_{g,CdS}$ at 2.5 eV. It shows a decrease in current density against an increase in voltage. It is noted that the same evolution is recorded on Fig.6-b while indicating a stability of the efficiency at the value $\eta_{CdS} = 27.66$ % with a decrease of EF_{CdS} in the piece of value $0.1\mu m$.

On the temperature interval between 300K and 350K for the CdS layer, Figs 7-a and 7-b illustrate the evolution of the characteristics of this layer under the condition of new parameters such as $E_{g,CdS} = 2.5$ eV and its thickness $0.1\mu m$. We notice the only significant increase in current density indicating a movement of the electron-holes, on the other hand there is a decrease in the other characteristics. For this test the η_{CdS} recorded efficiency is the order of 30 % instead of the 16 % illustrated in [11]–[13].

ZnO layer optimization when the thickness of CISSe is $20\mu m$, $E_{g,CISSe} = 1.7$ eV and the thickness of CdS is $0.1\mu m$ and $E_{g,CdS} = 2.5$ eV.

The test is taken at temperature of 300K respecting the following conditions: the thickness of CISSe is $20\mu m$ and $E_{g,CISSe} = 1.7$ eV and the thickness of CdS is $0.1\mu m$ and $E_{g,CdS} = 2.5$ eV. Figs.8-a and 8-b show the variation of the characteristics $J_{sc,ZnO}$; $V_{oc,ZnO}$; EF_{ZnO} ; η_{ZnO} of the main layer of the cell studied while putting the ZnO , $E_{g,ZnO}$ between 1 eV and 8 eV.

The Fig.8-a, above shows the stability of the voltage at the value 0.8436V during the variation of the $E_{g,ZnO}$. On the other hand we notice an increase in current density $J_{sc,ZnO}$ up to the value 45,89 mA/cm². On the other hand, Fig.8-b indicates a decrease in duality factor and an increase in efficiency until reaching a new value η_{ZnO} 30.41 % instead of 23 % illustrated in [14], [15]

The thickness of the ZnO layer is varied between $0.001\mu m$ and $0.1\mu m$ while keeping the optimal values found to check the variation on the four variables studied. We notice in Fig.9-a a decrease in $J_{sc,ZnO}$ as a function of the thickness and a stability of $V_{oc,ZnO}$ at the value 0.8436 V. As for Fig.9-b which notices an increase in efficiency up to a maximum value $\eta_{ZnO} = 30,47$ % by comparing with results illustrated in [16]. The factor of EF_{ZnO} has experienced a decrease of 40 %.

Figure 10 shows the action of the ZnO layer temperature variation on the characteristics of the CISSe/CdS/ZnO structure. The profile of the couples (J_{sc} , V_{oc}) and (FF , η) represented in figure.10-a and figure.10-b show a significant decrease in V_{oc} , FF and η against an increase in J_{sc} that expresses by the fact that the heat is lost due to release of an energy in $h\nu$ form. In despite of what happened, this remains encouraging because there is a little decrease in efficiency which not exceeding 2.98 %; value compared with those reviewed by the measures illustrated in references [17] [18].

Conclusion

In this article, the effect of thickness, gap energy and temperature have been demonstrated on the CISSe/CdS/ZnO layers to optimize the physical characteristics of the window layer CISSe, the buffer of CdS and absorption of ZnO. Using numerical simulation on the SCPAC-1D computer code, 12 tests were performed on the three layers. The results obtained show, on the basis of these parameters such as the Thickness of CISSe of $20\mu m$, $E_{g,CISSe} = 1.7$ eV, the thickness of CdS is $2.5\mu m$, $E_{g,CdS} = 1$ eV, thickness of ZnO is $0.001\mu m$ and $E_{g,ZnO} = 4$ eV and under a temperature of 300K, the improvement in the performance of the studied cell can reach 30.47 % for the absorbent layer, 30.07 % for the CdS layer and 28.8 % for the

window layer. These results remain satisfactory in comparison with the most recent measurements which were carried out on the same cell.

Abbreviations

Nomenclatures

E_g : Gap energy

FF : Fill factor

J_{sc} : Short circuit density.

V_{oc} : Open circuit voltage

h : Planc constant

ν : Frequency.

η : Efficiency

SCAPS-1D: One-dimensional Solar Cell Capacitance Simulator.

Declarations

Data Availability statement

The authors declare that there is no conflicts of interest regarding the publication of this paper.

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* **Ethics approval**

* **Consent to participate**

* **Consent for publication**

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* **Funding**

* **Authors' contributions**

References

- [1] G. Albalawneh and M. Ramli, "Review—Solution Processing of CIGSe Solar Cells Using Simple Thiol-Amine Solvents Mixture: A Review," *ECS J. Solid State Sci. Technol.*, vol. 9, no. 6, p. 061013, 2020, doi: 10.1149/2162-8777/aba4ee.
- [2] M. A. Ashraf and I. Alam, "Numerical simulation of CIGS, CISSe and CZTS-based solar cells with In₂S₃ as buffer layer and Au as back contact using SCAPS 1D," *Eng. Res. Express*, vol. 2, no. 3, 2020, doi: 10.1088/2631-8695/abade6.
- [3] L. Hu, H. Zhong, and Z. He, "Toxicity evaluation of cadmium-containing quantum dots: A review of optimizing physicochemical properties to diminish toxicity," *Colloids Surfaces B Biointerfaces*, vol. 200, no. February, p. 111609, 2021, doi: 10.1016/j.colsurfb.2021.111609.
- [4] S. Aseena, N. Abraham, and V. Suresh Babu, "Optimization of layer thickness of ZnO based perovskite solar cells using SCAPS 1D," *Mater. Today Proc.*, vol. 43, no. xxxx, pp. 3432–3437, 2020, doi: 10.1016/j.matpr.2020.09.077.
- [5] M. Zhou, W. Zhao, Q. Yan, and H. Fu, "Multiple interfacial polarization from 3D net-like ZnO@MWCNTs@NiFe₂O₄ nanocomposites as broadband microwave absorbers," *J. Alloys Compd.*, vol. 877, p. 160300, 2021, doi: 10.1016/j.jallcom.2021.160300.
- [6] D. A. Fentahun, A. Tyagi, and K. K. Kar, "Numerically investigating the AZO/Cu₂O heterojunction solar cell using ZnO/CdS buffer layer," *Optik (Stuttg.)*, vol. 228, no. December 2020, p. 166228, 2021, doi: 10.1016/j.ijleo.2020.166228.
- [7] M. A. Ghebouli, B. Ghebouli, R. Larbi, T. Chihi, and M. Fatmi, "Effect of buffer nature, absorber layer thickness and temperature on the performance of CISSe based solar cells, using SCAPS-1D simulation program," *Optik (Stuttg.)*, vol. 241, p. 166203, 2021, doi: 10.1016/j.ijleo.2020.166203.
- [8] S. Liu *et al.*, "Assembly of Cu–In–Sn–Se quantum dot–sensitized TiO₂ films for efficient quantum dot–sensitized solar cell application," *Mater. Today Energy*, vol. 21, p. 100798, 2021, doi: 10.1016/j.mtener.2021.100798.
- [9] O. Cojocaru-Mirédin *et al.*, "Intense sulphurization process can lead to superior heterojunction properties in Cu(In,Ga)(S,Se)₂ thin-film solar cells," *Nano Energy*, vol. 89, p. 106375, 2021, doi: 10.1016/j.nanoen.2021.106375.
- [10] S. Yu *et al.*, "Structure engineering of solution-processed precursor films for low temperature fabrication of CuIn(S,Se)₂ solar cells," *Sol. Energy*, vol. 220, pp. 796–801, May 2021, doi: 10.1016/j.solener.2021.03.079.
- [11] M. Su *et al.*, "Efficient SnO₂/CdS double electron transport layer for Sb₂S₃ film solar cell," *J. Alloys Compd.*, vol. 882, p. 160707, 2021, doi: 10.1016/j.jallcom.2021.160707.

- [12] H. Chen, Y. Lei, X. Yang, C. Zhao, and Z. Zheng, "Using a CdS under-layer to suppress charge carrier recombination at the Ag₂S/FTO interface," *J. Alloys Compd.*, vol. 879, p. 160348, 2021, doi: 10.1016/j.jallcom.2021.160348.
- [13] X. Wen, Z. Lu, G. C. Wang, M. A. Washington, and T. M. Lu, "Efficient and stable flexible Sb₂Se₃ thin film solar cells enabled by an epitaxial CdS buffer layer," *Nano Energy*, vol. 85, no. March, p. 106019, 2021, doi: 10.1016/j.nanoen.2021.106019.
- [14] T. Ouslimane, L. Et-taya, L. Elmaimouni, and A. Benami, "Impact of absorber layer thickness, defect density, and operating temperature on the performance of MAPbI₃ solar cells based on ZnO electron transporting material," *Heliyon*, vol. 7, no. 3, p. e06379, 2021, doi: 10.1016/j.heliyon.2021.e06379.
- [15] A. Soltanmoradi, F. Bakhtiargonbadi, H. Esfahani, and R. S. Moakhar, "Effects of microstructure and stoichiometry of ZnO electrospun seed layer on the photoelectrical and photoelectrochemical properties of ZnO nanorods grown on the FTO substrate," *Mater. Chem. Phys.*, vol. 267, no. March, p. 124718, 2021, doi: 10.1016/j.matchemphys.2021.124718.
- [16] I. Alam, R. Mollick, and M. A. Ashraf, "Numerical simulation of Cs₂AgBiBr₆-based perovskite solar cell with ZnO nanorod and P3HT as the charge transport layers," *Phys. B Condens. Matter*, vol. 618, no. March, p. 413187, 2021, doi: 10.1016/j.physb.2021.413187.
- [17] J. Ji, P. Sang, and J. H. Kim, "Improving the photoelectrochemical performance of spin-coated WO₃/BiVO₄/ZnO photoanodes by maximizing charge transfer using an optimized ZnO decoration layer," *Ceram. Int.*, vol. 47, no. 18, pp. 26260–26270, 2021, doi: 10.1016/j.ceramint.2021.06.035.
- [18] H. El Farri, M. Bouachri, M. Fahoume, A. Frimane, and O. Daoudi, "Theoretical simulation of ZnS buffer layer thin films with SCAPS-1D software for photovoltaic applications," *Chalcogenide Lett.*, vol. 18, no. 8, pp. 457–465, 2021.

Figures

Figure 1

CISSe/CdS/ZnO layer diagramme

Figure 2

CISSe characteristics evolution as a function of gap energy.

Figure 3

Thickness evolution on the characteristics of CISSe at $E_{g,\text{CISSe}} = 1.7 \text{ eV}$

Figure 4

Parameters evolution with thickness of 20 μm and $E_{g,\text{CISSe}} = 1.7 \text{ eV}$.

Figure 5

Variation of buffer layer characteristics.

Figure 6

Variation of J_{sc} , V_{oc} , FF, η with a $E_g, \text{CdS} = 2.5$ eV

Figure 7

Temperature effect on the conductive layer with an $E_{g,\text{CdS}} = 2.5 \text{ eV}$ and its thickness $0.1 \mu\text{m}$.

Figure 8

Evolution of the absorbent layer according to the new parameters found.

Figure 9

Effect of thickness on ZnO layer characteristics

Figure 10

Temperature evaluation on the absorbent cell.