JOURNAL OF NANO- AND ELECTRONIC PHYSICS | *ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ*
Vol. **15** No 2, 02025(5pp) (2023) | Том **15** № 2, 02025(5cc) (2023)

The Improved Performance with Reduction in Toxicity in CIGS Solar Cell Using Ultra-thin $BaSi_2$ BSF Layer

Km. Kanchan*, Anupam Sahu†, Shivangi Yadav‡

Department of Electronics and Communication Engineering,
Madan Mohan Malaviya University of Technology Gorakhpur, India

(Received 03 March 2023; revised manuscript received 18 April 2023; published online 27 April 2023)

In this article, the thin-film solar cell (TFSC) based on Copper-Indium-Gallium-Diselenide (CIGS) absorber layer and low-cost ultra-thin $BaSi_2$ Back Surface Field (BSF) with the framework of Al/SnO_2:F/buffer-layer/CIGS/$BaSi_2$/Mo/Substrate have been proposed. To enhance the performance and reduce the toxicity, the $Cd_{0.6}Zn_{0.4}S$ (alloy of CdS and ZnS) and ZnSe have been used as suitable buffer layers as a replacement for conventional toxic CdS buffer layers. The proposed TFSC also aims to be cost-effective, therefore the thickness of the CIGS layer has been optimized (varied from 0.1-1 μm). With the $Cd_{0.6}Zn_{0.4}S$ and ZnSe buffer layers, the proposed TFSC achieves the maximum conversion efficiency (CE) of 28.11 % and 27.72 %, respectively for the optimized CIGS thickness of 0.8 μm and $BaSi_2$ BSF layer thickness of 0.3 μm. Further, the proposed TFSC has been investigated for variation in defect density of the CIGS absorber layer. Additionally, the results obtained for the proposed TFSC show improvement in the performance from the previously reported CdS-based TFSC.

Keywords: CIGS, $Cd_{0.6}Zn_{0.4}S$, ZnSe, Thin-film solar cell, Conversion Efficiency, SCAPS-1D

DOI: 10.21272/jnep.15(2).02025 PACS number: 88.40.jm

1. INTRODUCTION

The fast depletion of traditional energy sources such as fossil fuels has prompted concern about the development of highly efficient, dependable, clean, and affordable renewable energy sources [1]. The solar cell is the best substitute to dominate the increase in worldwide power shortage crises [2]. Therefore, several research on different composite materials for thin-film solar cells (TFSC) namely a-Si, Cadmium-Telluride (CdTe), Copper-Zinc-Tin-Sulfide (CZTS), Copper-Indium-Gallium-Diselenide (CIGS), CZTSSe and organic resources has been carried to achieve the maximum conversion efficiency (CE) at relatively low fabrication cost [3-5].

The most commonly explored CIGS-based TFSC is relatively non-toxic compared to CdTe-based TFSC, due to the absence of toxic cadmium (Cd) material [6]. The CIGS offers high CE, and a high absorption coefficient (greater than 10^5 cm^{-1}) and hence can be considered a suitable candidate for reliable photovoltaic applications. The alloying of the CIGS material provides the tuning capability of the bandgap over the span of 1.04-1.67 eV [7]. Nevertheless, the high-cost value of CIGS solar cells is attributed to the deficiency of rare metals like Gallium (Ga) and Indium (In). Therefore, the CIGS absorber thickness must be reduced for low-cost fabrication of TFSC [8].

In the device structure of TFSC, the buffer layer plays an important role, as it secures the absorber layer from high-energy ions when sputtering from the window layer. Generally, the CIGS-based TFSCs frequently utilize CdS as a buffer layer [9], [10]. However, the materials based on Cd are toxic and hazardous to the environment [11]. Therefore, to reduce the toxicity $Cd_{1-y}Zn_yS$ buffer layer can be an attractive candidate, as its offers a tunable bandgap in the range 2.42 eV (CdS) and 3.62 eV (ZnS), putting it one step ahead of other materials [12]. Increasing Zn composition, the bandgap of $Cd_{1-y}Zn_yS$ increases enabling low wavelength photons through the device. The content of Zn in $Cd_{1-y}Zn_yS$ is varied to make it less toxic as much as possible and makes it suitable for photovoltaic devices. In this context, Moradi et al. [13] achieve the maximum CE of 21.32 % for the 20 % Zn in $Cd_{1-y}Zn_yS$/CIGS solar cell reach to a CE of around 21.32 %. Whereas, Hamri et al. [14], 60 % of Zn content archives high CE of 23.71 %.

The current losses in the CdS buffer layer are due to its narrow bandgap and parasitic absorption. Therefore, the higher bandgap material (Zinc oxides, selenide, and sulfides) is used as an alternative buffer layer of CdS in the extensive research. ZnSe has a greater bandgap than the CdS buffer layer which is the most promising material and a better alternative to CdS. However, higher bandgap materials face some interfacial electrical issues [15]. Also, another reason to use ZnSe instead of CdS is to reduce the toxicity of the CdS-based buffer layer.

In this work, we aim to improve the CE of TFSC with reduced cost and reduced use of toxic material. To achieve the aim, an ultra-thin $BaSi_2$-based Al/SnO_2:F/ buffer layer /CIGS/$BaSi_2$/Mo/ Substrate TFSC with $Cd_{0.6}Zn_{0.4}S$ and ZnSe buffer layers has been proposed. To reduce cost, the CIGS layer thickness has been varied from 0.1-1 μm. The proposed TFSCs have been optimized for different structural parameters. The TFSC structure has been

* kanchanjaiswal933@gmail.com
† anupam.or.sahu@gmail.com
‡ shivkarnika@gmail.com

simulated using a 1-D solar cell capacitance simulator (SCAPS-1D) to extract photovoltaics performance parameters such as open-circuit voltage (V_{oc}), Short circuit current density (J_{sc}), Fill Factor (*FF*) and Conversion efficiency (η). The proposed TFSC has been further investigated for the bulk-defect density of the absorber layer.

2. DEVICE STRUCTURE, METHODOLOGY AND MATERIAL PARAMETERS

The propsed TFSC device structure (Al/SnO_2:F/buffer layer/CIGS/$BaSi_2$/Mo/Substrate) is shown in Fig. 1, which consists of p^+-type $BaSi_2$ as a BSF layer, CIGS as a *p*-type absorber layer, $Cd_{0.6}Zn_{0.4}S$ and ZnSe as an *n*-type buffer layer and n^+-type SnO_2: F which serves as a window layer. Aluminum (Al) and Molybdenum (Mo) are two different metals used as front contact and back contact having the work function of 4.06 eV [16] and 4.95 eV [17], respectively. The buffer layer ($Cd_{0.6}Zn_{0.4}S$, ZnSe) constructs a *p-n* junction with the absorber layer (CIGS). The sunlight inserts through the window layer. The electron-hole pairs are generated at a *p-n* junction by the absorption of photons. Simulation of the proposed TFSC structure is under the standard solar spectrum AM 1.5 G with 1 KW/m^2 light intensity.

The performance of CIGS-based TFSC is investigated in various stages. Firstly, the thickness of the CIGS layer has been varied from 0.1-1 μm. For the optimized thickness, bulk defect density has been varied from 10^{12}-10^{16} cm^{-3}. In the simulation, the parameters listed in Table 2 have been used.

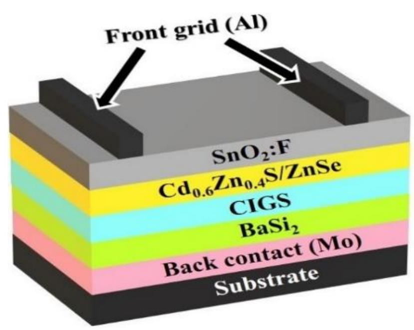

Fig. 1 – Schematic view of proposed TFSC

Table 1 – Electronic properties in general

NV	Valence Band effective Density of State, NV (cm^{-3})
ETV	The thermal velocity of the electron, (cm·s^{-1})
HTV	The thermal velocity of the hole, (cm·s^{-1})
MDN	Mobility of electron, μ_e (cm^{2}V^{-1}s^{-1})
MDP	Mobility of hole, μ_h (cm^{2}V^{-1}s^{-1})
ND	Donor density, N_D (cm^{-3})
NA	Acceptor density, N_A (cm^{-3})
NT	Bulk defect density, N_t (cm^{-3})
TH	Layer thickness (μm)
EG	Band gap, E_g (eV)
CHI	Electron affinity, χ (eV)
DC	Dielectric Permittivity, ε_r
NC	Conduction Band effective Density of State, N_c (cm^{-3})

3. RESULT AND DISCUSSION

The proposed CIGS-based TFSC configuration (Al/SnO_2:F/ buffer layer /CIGS/$BaSi_2$/Mo/ Substrate) with $Cd_{0.6}Zn_{0.4}S$ and ZnSe as a buffer layer has been examined to enhance the photovoltaic performance. The parameter variation of the proposed TFSC based on CIGS is depicted in Figs. 2 and 3. The following section illustrates the output photovoltaic parameters (V_{oc}, J_{sc}, *FF* and η) for the optimum configuration of thickness and bulk defect density of the absorber layer at the operating temperature of 300 K.

Table 2 – The physical parameter of materials used for simulation

Parameters (unit)	n^+-SnO_2:F [8]	*n*-ZnSe [15]	*n*-$Cd_{0.6}Zn_{0.4}S$ [12]	*p*-CIGS [15]	p^+-$BaSi_2$ [8]
TH	0.05	0.05	0.05	0.1-1.0	0.3
EG	3.6	2.9	2.83	1.2	1.3
CHI	4.0	4.2	4.26	4.0	3.3
DC	9.0	10	9.23	13.6	11.17
NC	2.2×10^{18}	2×10^{18}	2.1×10^{18}	2×10^{17}	2.6×10^{19}
NV	1.8×10^{19}	1.8×10^{19}	1.7×10^{19}	1.5×10^{19}	2×10^{19}
ETV	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
HTV	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
MDN	100	70	70	100	820
MDP	25	3	20	25	100
ND	1×10^{19}	5.5×10^{7}	1×10^{16}	0	0
NA	0	0	0	2×10^{16}	5×10^{18}
NT	1×10^{15}	1×10^{15}	1×10^{15}	2.5×10^{14}	1×10^{15}
Defect type	SA	SA	SA	SD	SD

3.1 Impact of CIGS Absorber Layer Thickness on the Photovoltaic Performance

The impact of varying the thickness of the absorber layer on the photovoltaic parameter of solar cell is examined by simulation of two different structures based on $Cd_{0.6}Zn_{0.4}S$/CIGS and ZnSe/CIGS. For each structure, the absorber layer thickness is tuned from 0.1-1 μm, the buffer layer thickness is 0.05 μm. Fig. 2 depicts the influence of variation of CIGS layer thickness on V_{oc}, J_{sc}, *FF* and CE (η). For the structure $Cd_{0.6}Zn_{0.4}S$/CIGS the decrease in V_{oc} from 0.97 to 0.89 V and a considerable rise of J_{sc} is noticed from 23.40 mA/cm^2 to 41.87 mA/cm^2, whereas *FF* reduced from 80.66 % to 75.09 % and CE goes up from 18.21 % to 28.11 % and for the structure ZnSe/CIGS the V_{oc} has been dropped from 0.96 V to 0.89 V and a noteworthy enhancement in J_{sc} is noticed from 22.26 mA/cm^2 to 41.34 mA/cm^2, whereas a reduction in *FF* from 80.32 % to 75.11 % and CE increases from 17.20 % to 27.75 % as given in Fig. 2. The increase in reverse saturation current density (J_0), promotes the charge carrier recombination, and is responsible for the reduction in V_{oc}.

The increase in short circuit current is mostly owing to the fact that an absorber layer having a larger thickness permits more photons of long-wavelength to be absorbed, resulting in increased carrier production [1]. The internal resistance increases when the absorber layer thickness is increased. The depletion was accelerated as a result of the

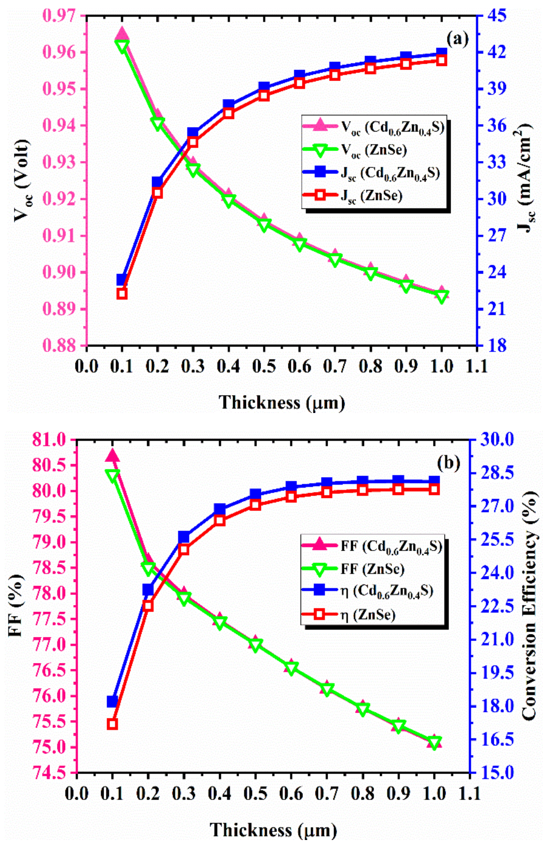

Fig. 2 – Effect of absorber layer thickness variation on photovoltaic parameter: (a) V_{oc} and J_{sc}, (b) Fill Factor and Conversion efficiency (η)

increased resistance, lowering the Fill factor [18]. Two aspects that need to be kept in the simulation study to determine the CE of TFSC are light absorption and carrier transfer. Light absorption becomes a major factor with a thin absorber layer since all carriers can radially reach the associated electrode. Light absorption becomes saturated when the thickness of the absorber layer crosses the threshold value, and carrier moments correspond to a key factor. The relation between these two parameters draws a conclusion which can be seen in Fig. 2(b) that increasing thickness above 0.8 μm has no more effect on CE of CIGS based TFSC. The TFSC having very thin CIGS absorber layer corresponds to low CE as the CIGS would not be able to absorb all the incoming light falling on its surface. In the same way, the absorber layer having a thickness greater than the optimum value results in increased recombination of created carriers as the journey of photo-produced carriers gets longer than earlier.

3.2 Impact of Bulk Defect Density of CIGS Absorber Layer on the Photovoltaic Performance

The bulk defect density of single-donor-type changed from 1×10^{12} to 1×10^{16} cm^{-3} of the CIGS layer, to study the impact of variation on the performance parameter of TFSC, while other layers have the same defect densities as mentioned in Table 2. Fig. 3 depicts the affect of different defect density levels on the TFSC performance characteristics. As the defect density rises, the values of V_{oc}, J_{sc}, FF and CE reduces for both structures. For ZnSe/CIGS structure; J_{sc} drops from 40.73 mA/cm^2 to 38.91 mA/cm^2, V_{oc} drops from 1.05 V to 0.75 V and FF drops from 84.28 % to 61.67 %. As a result, the CE

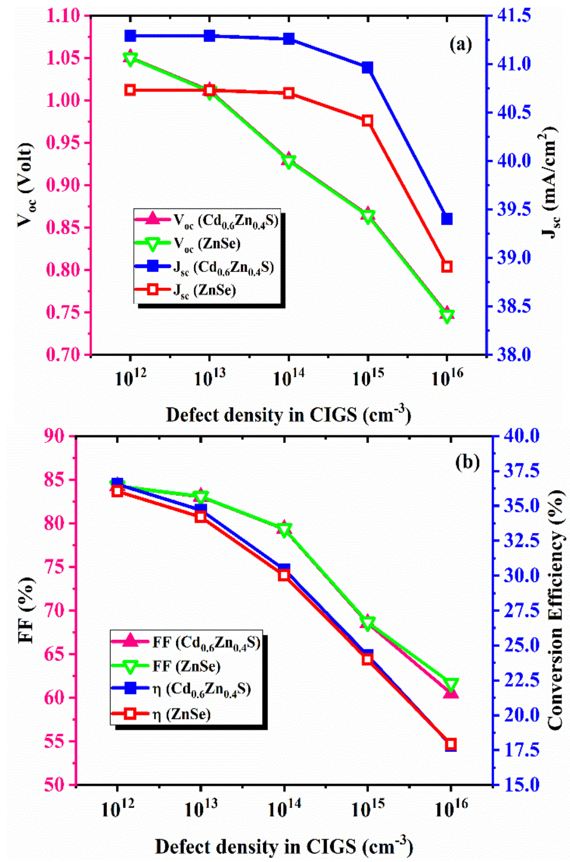

Fig. 3 – Effect of bulk defect density variation of absorber layer on photovoltaic parameter: (a) V_{oc} and J_{sc}, (b) Fill Factor and Conversion efficiency (η)

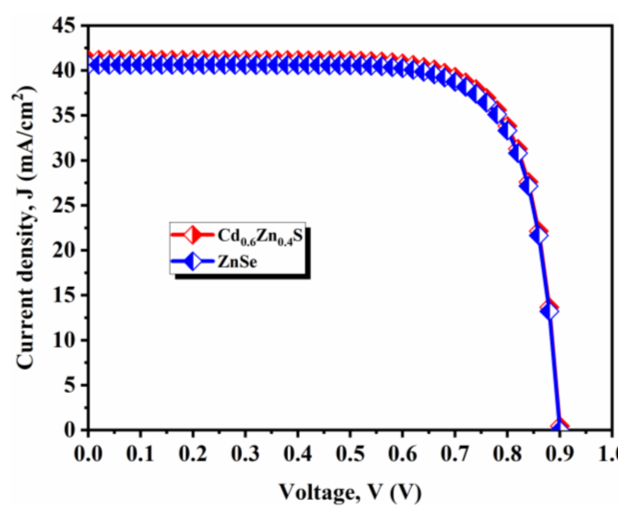

Fig. 4 – The *J-V* characteristic of the proposed TFSC

drops from 36.04 % to 17.92 %, and similarly for $Cd_{0.6}Zn_{0.4}S$/CIGS structure J_{sc} drops from 41.29 mA/cm^2 to 39.41 mA/cm^2, V_{oc} drops from 1.05 V to 0.75 V, and *FF* drops from 84.27 % to 60.51 %, and CE from 36.55 % to 17.83 %. With the increase in defect density, the risk of electron-hole recombination before the carriers approach the junction and produce current also rises. It means that the higher the defect density is, the lower rate of electron-hole pair formation will be. Defects can quickly degrade photovoltaic performance, reducing the CE of TFSCs. To improve the proposed TFSC output, the defect density should be kept to a minimum value.

Using optimized parameters, obtained current density–voltage (*J-V*) curve is illustrated in Fig. 4. The thickness of 0.05 μm is used for $Cd_{0.6}Zn_{0.4}S$, ZnSe, and FTO layer also 0.8 μm and 0.3 μm are employed for CIGS and $BaSi_2$ layer, respectively.

Table 3 – Summary and comparison of photovoltaic performance of proposed TFSC with reported CIGS based TFSC

Structure (Buffer/Absorber)	V_{oc} (volt)	J_{sc} (mA/cm^2)	*FF* (%)	η (%)	Reference No.
CdS/CIGS	0.74	34.47	83.09	21.30	[9]
CdS/CIGS	0.75	38.7	79.18	22.92	[19]
CdS/CIGS	0.80	35.64	84.75	24.17	[7]
CdS/CIGS	0.88	36.09	86.49	27.65	[20]
ZnSe/CIGS	0.90	40.65	75.76	27.72	Proposed
$Cd_{0.6}Zn_{0.4}S$/CIGS	0.90	41.21	75.76	28.11	Proposed

4. CONCLUSION

The performance of a CIGS-based TFSC has been thoroughly explored in this study. By utilizing two different buffer layers: $Cd_{0.6}Zn_{0.4}S$ and ZnSe, the output performance parameters are determined by varying the thickness of the absorber layer and bulk defect density. SnO_2: F (FTO) window layer, buffer layer $Cd_{0.6}Zn_{0.4}S$, and ZnSe have a thickness of 0.05 μm, and the CIGS absorber layer has a thickness of 0.8 μm. Structure ($Cd_{0.6}Zn_{0.4}S$/CIGS) for a defect of 2.5×10^{14} cm^{-3} has CE (η) of 28.11%, with J_{sc} of 41.21 mA/cm^2.The structure (ZnSe/CIGS) with the same defects represents CE of 27.72 % with J_{sc} of 40.65 mA/cm^2. *FF* is the same for both structures 75.76 % with V_{oc} of 0.90 Volts. The toxicity of CIGS solar cells is being reduced by 40 % by substituting CdS with $Cd_{0.6}Zn_{0.4}S$, and with ZnSe as a buffer layer, the toxicity is negligible. This study's optimization may result in the generation of a highly efficient and innocuous CIGS-based TFSC. Its ultrathin layer architecture led to its cost-effectiveness.

ACKNOWLEDGEMENT

We would like to acknowledge the use of the SCAPS-1D program that was developed by Marc Burgelman at the University of Gent, Belgium.

REFERENCES

1. N. Singh, A. Agarwal, M. Agarwal, *Sol. Energy* **208**, 399 (2020).
2. K.L. Chopra, P.D. Paulson, V. Dutta, *Prog. Photovolt. Res. Appl.* **12** No 2-3, 69 (2004).
3. A. Mohammad Bagher, *Am. J. Opt. Photon.* **3** No 5, 94 (2015).
4. S. Rao, A. Morankar, H. Verma, P. Goswami, *J. Appl. Chem.* **2016**, 1 (2016).
5. M.E.D. Abd Elhalim Benzetta, Mahfoud Abderrezek, *J. Nano-Electron. Phys.* **14** No 2, 02012 (2022).
6. G.A.M. Hashmi, W.A.A. Syed, M. Hayat, W.H. Shah, N.A. Shah, *Mater. Res. Exp.* **6** No 10, 106440 (2019).
7. R. Prasad, A.K. Das, U.P. Singh, *Appl. Phys. A: Mater. Sci. Process.* **127** No 2, 1 (2021).
8. S.R.I. Biplab, M.H. Ali, M.M.A. Moon, M.F. Pervez, M.F. Rahman, J. Hossain, *J. Comput. Electron.* **19** No 1, 342 (2020).
9. H. Heriche, Z. Rouabah, N. Bouarissa, *Int. J. Hydrogen Energy* **42** No 15, 9524 (2017).
10. H. Heriche, Z. Rouabah, N. Bouarissa, *Optik (Stuttg)* **127** No 24, 11751 (2016).
11. F.T. Nya, G.M.D. Kenfack, *Thin-film Solar Cells Performances Optimization: Case of Cu (In, Ga) Se_2-ZnS* in *Solar Cells: Theory, Materials and Recent Advances* (Ed. by A.M. Elseman) (IntechOpen: 2012).
12. T. Hossain, et al., *Superlattice. Microst.* **161**, 107100 (2021).
13. M. Moradi, R. Teimouri, M. Zahedifar, M. Saadat, *Optik (Stuttg)* **127** No 8, 4072 (2016).
14. Y.Z. Hamri, Y. Bourezig, M. Medles, M. Ameri, K. Toumi, I. Ameri, Y. Al-Douri, C.H. Voon, *Sol. Energy* **178**, 150 (2019).
15. J. Qu, L. Zhang, H. Wang, X. Song, Y. Zhang, H. Yan, *Opt. Quant. Electron.* **51** No 12, 383 (2019).
16. M.M.A. Moon, M.F. Rahman, J. Hossain, A.B.M. Ismail, *Adv. Mater. Res.* **1154**, 102 (2019).
17. M. Sijanur, R. Robin, M. Mansoor, M. Rasmi, *2016 3rd International Conference on Electrical Engineering and Information Communication Technology (ICEEICT)* (2016).
18. G.M.M.W. Bissels, et al., *Sol. Energy Mater. Sol. C.* **130**, 605 (2014).
19. M.W. Bouabdelli, F. Rogti, N. Lakhdar, M. Maache, *J. Nano-Electron. Phys.* **12** No 3, 03002 (2020).
20. Y. Osman, M. Fedawy, M. Abaza, M.H. Aly, *Opt. Quant. Electron.* **53** No 5, 245 (2021).

Покращена продуктивність зі зниженням токсичності сонячної батареї CIGS із використанням ультратонкого шару $BaSi_2$ BSF

Km. Kanchan, Anupam Sahu, Shivangi Yadav

Department of Electronics and Communication Engineering,
Madan Mohan Malaviya University of Technology Gorakhpur, India

У цій статті представлено тонкоплівковий сонячний елемент (TFSC) на основі поглинаючого шару міді-індія-галію-диселеніду (CIGS) і недорогого ультратонкого $BaSi_2$ Back Surface Field (BSF) із каркасом Al/SnO_2F/буферний шар/CIGS/$BaSi_2$/Mo/підкладка були запропоновані. Щоб підвищити ефективність і зменшити токсичність, $Cd_{0.6}Zn_{0.4}S$ (сплав CdS і ZnS) та ZnSe були використані як відповідні буферні шари замість звичайних токсичних буферних шарів CdS. Запропонований TFSC також повинен бути економічно ефективним, тому товщину шару CIGS було оптимізовано (варіюється від 0,1-1 мкм). З буферними шарами $Cd_{0.6}Zn_{0.4}S$ and ZnSe запропонований TFSC досягає максимальної ефективності перетворення (CE) 28,11 % і 27,72 % відповідно для оптимізованої товщини CIGS 0,8 мкм і шару $BaSi_2$ BSF 0.3 мкм.Крім того, запропонований TFSC був досліджений на зміну щільності дефектів поглинаючого шару CIGS. Крім того, результати, отримані для запропонованого TFSC, показують покращення продуктивності порівняно з раніше зареєстрованим TFSC на основі CdS.

Ключові слова: CIGS, $Cd_{0.6}Zn_{0.4}S$, ZnSe, Тонкоплівковий соняний елемент, Ефективність перетворення, SCAPS-1D.