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Research Article

Modeling of a Tandem Solar Cell Structure Based on CZTS and CZTSe Absorber Materials

Hayat ARBOUZ*

University of Blida1, Faculty of Sciences, Physics Department, 09000, Blida- Algeria
* **Corresponding Author** : arbouzhayet@yahoo.fr **ORCID:** 0000-0003-2780-5215

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Abstract:

In this paper, we simulated a double junction cell based on top CdS/Cu_2ZnSnS_4 cell, stacked on a bottom $CdS/Cu_2ZnSnSe_4$ cell. We started by studying the perfomance of the bottom solar cell, based on the copper zinc tin selenide $Cu_2ZnSnSe_4$ (CZTSe) absorber. Then, we evaluated the photovoltaic parameters of the tandem cell at the optimized thickness of the copper zinc tin sulfide Cu_2ZnSnS_4 (CZTS) absorber of the top cell, where the top and bottom cells deliver the same photocurrent density. We achieved A maximum efficiency of 24.68% with an open circuit voltage of 1.33 V and a photocurrent density of 16.54 mA/cm² for the thicknesses 413.8 nm and 2 µm of CZTS and CZTSe absorbers, respectively. İn order to improve power conversion efficiency, light trapping effects was studied. The use of randomly textured top cell absorber allows the reduction of its thickness to 270 nm. An efficiency of 24.71% was then obtained. Finally, the effect of replacing the toxic CdS buffer absorber with the ZnS material was investigated.

1. Introduction

It is difficult to predict the world economic and technological development without using renewable energy sources [1]. Photovoltaic technology has experienced considerable development since its emergence. Silicon technology remains dominant and currently shares about 85% of the total photovoltaic market [2]. The other sectors based on thin films such as $CuInGaSe_2$ (CIGS) have experienced a remarkable progress, and have reached efficiency records exceeding 22% [3]. However, due to the use of rare and expensive metals [4], Kestrite materials have emerged as one of the best candidates for replacing the CIGS absorber material [5]. Kestrite semiconductors, such as Cu_2ZnSnS_4 (CZTS), $Cu_2ZnSnSe_4$ (CZTSe), and $Cu_2ZnSn(S,Se)_4$ (CZTSSe) have very attractive properties as they are eco-friendly, with high absorption coefficient [6],in addition to direct and tunable band gap energy between 1 eV and 1.5 eV [7]. Nevertheless, solar cells based on these materials suffer from poor efficiency in addition to large V_{oc} deficit [8]. Thus, using an improved device is required. In order to achieve higher efficiency and to increase the open circuit voltage V_{oc}. Multi-junction tandem structures offer this possibility. A tandem solar cell is a stack of two or more p-n junctions with band gap energies, which decreases in the depth direction from the top surface [9]. The tandem concept has been well established with thin film solar cells based on III-V compound semiconductors and has been used for space applications. Several tandem structures based on CZTS/CZTSe and perovskite/CZTS multi-junctions have been suggested [10].

In this paper, a dual-junction solar cell based on CZTS and CZTSe absorbers has been simulated. İndeed, The performance of the single CZTSe based cell which represents the bottom part of the studied tandem cell, was primarily examined. Moreover, the absorber thickness has been optimized in order to reach the best efficiency. Furthermore, the thickness of the CZTS absorber of the top cell has been adjusted to achieve the density of current match of top and bottom cells. Then, the light trapping effects was invistigated, through using a back mirror in the bottom cell and a randomly textured surface absorber geometry.

Finaly, replacing the toxic CdS buffer by ZnS material on the device was studied.

2. Tandem Cell Structure

Figure.1 illustrates the targeted tandem cell structure, where are connected in series two cells based on 1.5 eV-CZTS and 1 eV-CZTSe absorbing materials. The top cell architecture consists of the stacking of the following layers ATO/n-ZnO/CdS/CZTS, according to the design reported by Shin [11] , while the bottom cell consists of n-ZnO/CdS/CZTSe.

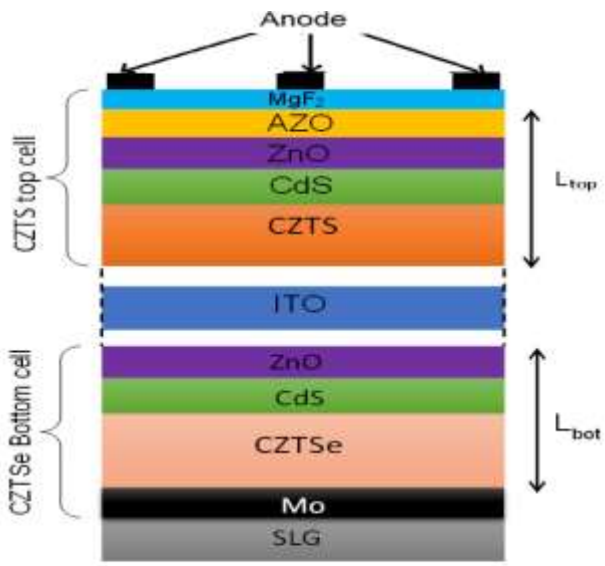

Figure 1. *CZTSe/CZTS Tandem Solar Cell Structure.*

In this simulated device, an ITO tunnel junction was introduced due to its low resistance and high transparency.

3. Simulation Model

In order to calculate the photocurrent densities generated by top and bottom cells, the wavelength-dependent absorption coefficient of the different structure layers was calculated by the well-known expression provided by Tauc and Al model [12]. The photo generated current densities were calcutalted using the equations expressed below, assuming perfect EQE [13]:

$$J_{ph,top} = q.\int_0^{+\infty} \frac{\lambda}{hc}.F(\lambda).\alpha_{top}(\lambda).d\lambda \qquad (1)$$

$$J_{ph,bot} = q.\int_0^{+\infty} \frac{\lambda}{hc}.F(\lambda).(1-\alpha_{top}(\lambda)).\alpha_{bot}(\lambda).d\lambda \qquad (2)$$

F(λ) represents the wavelength-dependent irradiance spectrum, *h* is the constant of Planck and *c* is the light velocity.

In this work, the absorptivity was calculated according to the model reported by [14]. For planar top absorber surface, the absorptivity $\alpha_{top}(\lambda)$ of top cell and that of bottom cell $\alpha_{bot}(\lambda)$ are expressed, according to equation 3 (not clear). and equation 4. below,as functions of absorption coefficients of CZTS and CZTSe materials, respectively.:

$$\alpha_{top}(\lambda) = 1 - \exp(-\alpha_{CZTS}(\lambda).L_{top}) \qquad (3)$$

$$\alpha_{bot}(\lambda) = 1 - \exp(-i.\alpha_{CZTSe}(\lambda).L_{bot}) \qquad (4)$$

i=1, if there is no back mirror in bottom cell; while *i=2*, in the case of back mirror presence.
L_{top} and L_{bot} represent top and bottom cell thicknesses respectively.
In the case of randomly textured surface absorber, the expressions become:

$$\alpha_{top}(\lambda) = 2.\int_0^{\pi/2}\left(1-e^{\alpha_{CZTS}(\lambda).\frac{L_{top}}{cos\theta}}\right).cos\theta.sin\theta.d\theta \quad (5)$$

$$\alpha_{bot}(\lambda) = \frac{4.n_{ref}^2.\alpha_{CZTSe}(\lambda).L_{bot}}{1+4.n_{ref}^2.\alpha_{CZTSe}(\lambda).L_{bot}} \qquad (6)$$

n_{ref} is the CZTSe refractive index.
Ferhati has reported that saturation current densities of both CZTS and CZTSe cells could be expressed as follows [15] :

$$J_s = q.Nc_{Abs}.Nv_{Abs}.(\frac{1}{Na}.\sqrt{\frac{Dp}{\tau p}}.\exp\left(\frac{-E_{g,Abs}}{V_{th}}\right) + q.Nc_{Buff}.Nv_{Buff}(\frac{1}{Nd}.\sqrt{\frac{Dn}{\tau n}}.\exp(\frac{-E_{g,Buff}}{V_{th}})) \qquad (7)$$

$N_{v\,Abs}$, Nc_{Abs} are the effective densities of states for each absorber.
N_a,N_d represent doping concentrations of the absorber and buffer materials respectively.
$E_{g,\ Abs}$ and $E_{g,\ Buff}$ are the band gap energies of the absorber and the buffer layers.

The photovoltaic parameters were calculated using the expressions reported in literature.
The open circuit voltage of a tandem cell is the sum of individual open circuit voltages of the top and bottom cells. However, the total current density is limited to the lower value associated with the sub cells [16].

4. Results and Discussions

İn this study, photovoltaic parameters such as V_{oc}, J_{ph} and efficiency of the single CZTSe cell wich was used as the lower part of the tandem cell were fistly

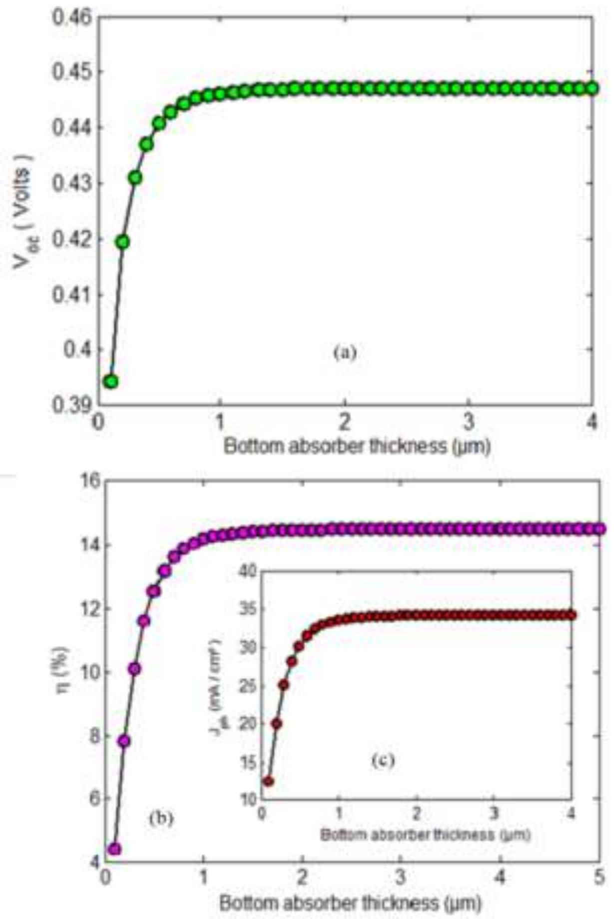

Figure 2. *V_{oc}, J_{ph} and η of Single-CZTSe solar cell as function of CZTSe thickness.*

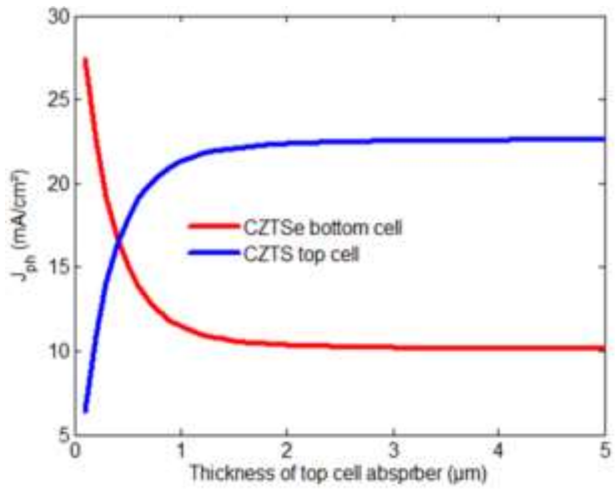

Figure 3. *Photocurrent Density as Function of Top Cell Absorber thickness.*

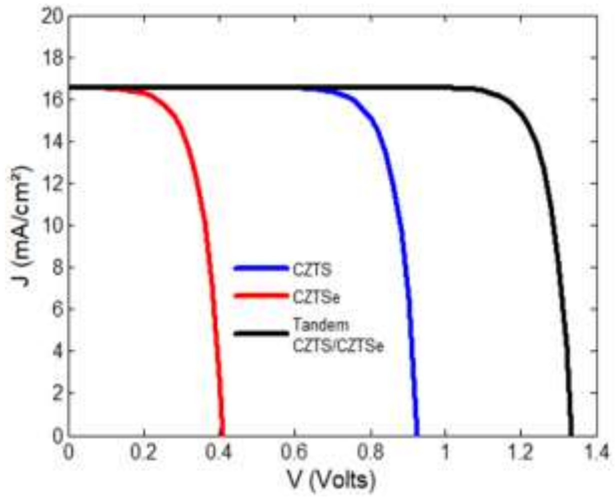

Figure 4. *J(V) Characteristics of CZTSe,CZTS and CZTS/CZTSe Tandem cells.*

examined as function of the absorber thickness augmentation. Figure.2 shows the obtained results. An optimal thickness of 2 µm was considered for where a maximum efficiency of 14.46 % was reached with J_{ph} = 34.18 mA/cm² and V_{oc}= 0.4472V. The matched photocurrent density condition should be achieved in a tandem cell in order to avoid unnecessary losses. The current matching analysis represented on figure.3 shows that both cells match with a value of J_{ph} = 16.54 mA /cm² for a top cell absorber thickness of about 414 nm.

The results of this study regarding the optimised absorber thickness determined above show an achieved efficiency of 24.68%, with an open circuit voltage of 1.33 V, a short circuit current density of 16.56 mA/cm² and a fill factor of 78.2% .

The resulted current density-voltage characteristics of top, bottom and of the whole tandem cells are shown in figure.4.

Light trapping techniques are generally used in order to improve the performance of the cells. In this section, we have replaced the previous CZTS absorber by a randomly textured surface of the same material, for trapping more light and increase absorption.

The absorptivities of top and bottom cells were calculated according to equation 5. and equation 6.

In this part of the study,the thickness was also determined according to the current match condition. The results showed that current densities of top and bottom cells share the same value at a thickness of 269.8 nm, which is thinner than the flat surface absorber studied above. An efficiency of 24.71 % was obtained with an open circuit voltage of 1.33 V, a fill factor of 78.2 % and a short current density of 16.56 mA/cm².

CdS deposited by chemical bath CBD [17,18] is the most used material as a buffer layer in CIGS and CZTS solar cells. However, this material contains cadmium which is highly toxic.To conclude, this study investigated the effect of replacing the CdS buffer material by ZnS in the tandem device.

The results showed that 1.5 µm was the optimal thickness of the CZTSe bottom absorber. The photocurrent density of top and bottom cells matches with 16.67 mA/cm² at a thickness of 410 nm of the CZTS absorber of the top cell. The current density-.

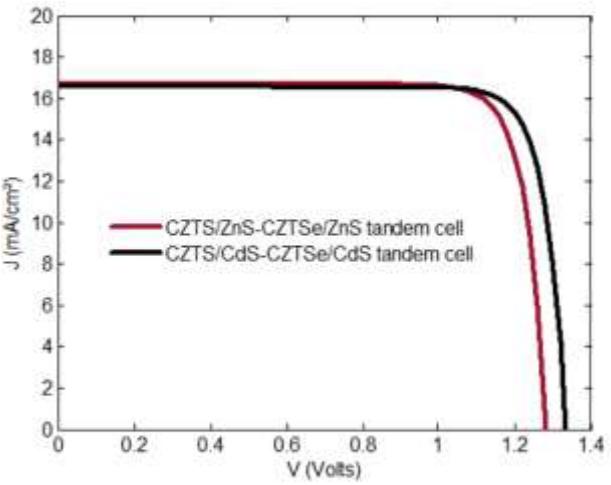

Figure 5. *J(V) Characteristic of ZnS Buffered CZTS/CZTSe Tadem Cell.*

voltage characteristics of the ZnS and CdS buffered tandem solar cells are represented in figure.5.

The results of the simulation showed that CZTS/CZTSe tandem solar cell based on ZnS buffer material reached a 23.83 % efficiency with 1.28 V open circuit voltage, 16.67 mA/cm² short circuit current density and 78% fill factor.

The numerical values of the photovoltaic parameters of the structures simulated in our work have been grouped in table 1.

Table 1. *Results of the Simulation.*

Structure	V_{oc} (V)	J_{sc}(mA/cm²)	FF (%)	η (%)
CZTSe Cell	0.4472	34.18	78.5	14.46
CZTS/CZTSe Tandem Cell	1.335	16.56	78.2	24.68
Textured-CZTS/CZTSe Tandem cell	1.336	16.56	78.2	24.71
CZTS/CZTSe Tandem cell, ZnS buffer	1.28	16.67	78.0	23.83

The results indicate the superiority of the tandem device based on kestrite absorbers to achieve high efficiencies compared to single-junction kestrite cells.

5. Conclusions

In this study, a tandem solar cell based on kestrite CZTS and CZTSe absorbers, was investigated. The simulation results showed that both top and bottom cells matche with a photocurrent density value of 16.54 mA / cm² when top cell CZTS absorber thickness is 414 nm. An efficiency of 24.68 % was achieved with an open circuit voltage of 1.33 V and a fill factor of 78.2%. The use of randomly textured CZTS top cell absorber surface allowed the reduction of its thickness to 270 nm. An efficiency of 24.7% was reached with V_{oc} = 1.33 V and J_{ph} = 16, 56 mA / cm². Finally, the use of ZnS buffer as an alternative material to toxic CdS in the tandem structure was investigated. The results showed that for a thickness of 1.5 µm of CZTSe and a thickness of 410 nm of CZTS, an efficiency of 23.83% is obtained with Voc = 1.28 V , Jph = 16, 67 mA / cm², and FF = 78%.

This work has demonstrated the ability of the tandem structure device based on kestrite materials absorber material not only to achieve efficiencies close to 25% but also to improve the open circuit voltage value.

Author Statements:

- **Ethical approval:** The conducted research is not related to either human or animal use.
- **Conflict of 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
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- **Data availability statement:** The data that support the findings of this study are available on request from the corresponding author. The data are not publicly available due to privacy or ethical restrictions.

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