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

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Abstract

İn this paper a kestrite double junction tandem solar cell based on a CdS/Cu_2ZnSnS_4 top cell stacked on $CdS/Cu_2ZnSnSe_4$ bottom cell has been simulated. Firstly, the performance of the bottom cell was investigated against the variation of the CZTSe absorber thickness. The performance of the tandem cell was determined according to the optimized CZTS top cell absorber thickness for which current match condition of top and bottom sub cells is reached. A maximum efficiency of 24.68 % with 1.33 V open circuit voltage was achieved for 16.54 mA/cm² density of current, 413.8 nm thick CZTS top cell absorber and 2µm thick CZTSe bottom cell absorber. İn order to improve power conversion efficiency, light trapping effects have been investigated in this work. The use of back mirror in the bottom sub cell has led to a double absorption in the CZTSe layer allowing the increase of efficiency up to 24.8%. This work also demonstrated that the use of randomly textured top cell absorber allows the reduction of its thickness to 270 nm. An efficiency of 24.71% was than obtained. Finally, the effect of replacing the toxic CdS buffer absorber with the ZnS material was investigated.

1 Introduction

Photovoltaic technology has experienced considerable development since its appearance. silicon technology remains dominant and currently share about 85% of the total photovoltaic market (Kumar, 2015), the other sectors based on thin films such as $CuInGaSe_2$ (CIGS) have experienced remarkable progress, and have reached efficiency records exceeding 22% (Jackson, 2016). However, due to the use of rare and expensive metals (Saha, 2017), Kestrite materials have emerging as one of the best candidates for replacing the CIGS absorber material (Suryawanshi, 2013).

Kestrite semiconductors such as Cu_2ZnSnS_4 (CZTS), $Cu_2ZnSnSe_4$ (CZTSe), and $Cu_2ZnSn(S,Se)_4$ (CZTSSe) have very attractive properties (Wang, 2013) with direct and tunable band gap energy between 1 eV and 1.5 eV (Yin, 2015) . However, solar cells based on these materials suffers from poor efficiency (Kim, 2014), and (Green, 2019), in addition to large V_{oc} deficit (Garud, S., 2017).

Thus, it becomes essential to utilize an improved device 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 (Gupta, G.K.).

Several tandem structures based on CZTS/CZTSe and perovskite/CZTS multi-junctions have been proposed (Todorov, 2014).

In this paper, a dual-junction solar cell based on CZTS and CZTSe absorbers was simulated. The performance of the single CZTSe based cell, which represents the bottom part of the studied tandem cell was firstly investigated. The absorber thickness was optimized in order to reach the best efficiency. The thickness of the CZTS absorber of the top cell was adjusted to achieve the density of current match of top and bottom cells .

Light trapping effects such as using back mirror in the bottom cell and considering randomly textured surface absorber geometry were investigated.

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

2 Tandem Cell Structure

Figure 1 illustrates the considered tandem cell structure, in which 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 empilement of the following layers ATO/n-ZnO/CdS/CZTS, according to the design reported by (Shin, B., 2013) while the bottom cell consists of n-ZnO/CdS/CZTSe .

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

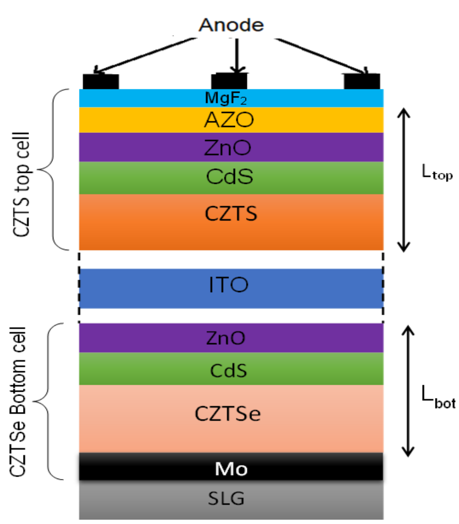

Figure 1: CZTSe/CZTS tandem solar cell structure

3 Model Description

In order to calculate the photocurrent densities generated by top and bottom cells, the wavelength-dependent absorption coefficient of the different layers of the structure was calculated by the well-known expression provided by Tauc and Al model (Tauc, 1972). The photo generated current densities were calculated assuming perfect EQE (White, 2014):

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

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

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

$\alpha_{top,bot}$ (λ) is the absorptivity of top/bottom cell.

In this work, the absorptivity of both sub cells were calculated according to the model reported in (Onno, 2016). For planar top absorber surface, the absorptivity $\alpha_{top}(\lambda)$ of top cell and that of bottom cell $\alpha_{bot}(\lambda)$ are expressed as follows:

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

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

i=1, if there is no back mirror in bottom cell; while i=2, in the case of presence of a back mirror.

$L_{top,bot}$: top/bottom cell thickness.

In the case of randomly textured surface absorber, the expressions become:

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

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

n_{ref} : CZTSe refractive index.

The saturation current densities of both CZTS and CZTSe cells could be expressed as follows (Ferhati, H., 2019) :

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

Nv_{Abs} , Nc_{Abs} : Absorber effective densities of states.

Na : doping concentration absorber, Nd : Doping concentration buffer.

Eg_{Abs} , Eg_{Buff} : band gap energies of the absorber and the buffer layers.

The current voltage characteristics associated with each cell is expressed by :

$$J(V) = J_{ph} + J_s.(1 - e^{\frac{qV}{nkT}}) \quad (8)$$

k: Boltzmann constant. T: cell temperature, n : ideality factor.

The electrical parameters of each cell are given as follows.

The solar cell open circuit voltage is calculated using :

$$V_{oc} = \frac{nkT}{q}.\ln(\frac{J_{ph}}{J_s} + 1) \quad (9)$$

The fill factor is defined by the ratio :

$$FF = \frac{J_m \cdot V_m}{V_{oc} \cdot J_{ph}} = \frac{P_m}{V_{oc} \cdot J_{ph}} \tag{10}$$

P_m is the maximum power density delivered which is the combination of maximum operation voltage V_m and current density J_m of the cell.

The efficiency is defined as:

$$\eta = \frac{P_m}{P_{inc}} \tag{11}$$

Where, P_{inc} is the incident power density. The open circuit voltage of tandem cell is equal to the summation of individual V_{oc} of top and bottom cells. However, the total density of current is limited to the lower value associated with the sub cells (Elbar, 2015).

4 Simulation Approach and Discussion

In this study, the electrical parameters such as V_{oc}, J_{ph} and efficiency η of the single CZTSe cell were examined firstly as function of the absorber thickness, which was varied from 0.1 µm to 4 µm. Figure 2 shows the obtained results.

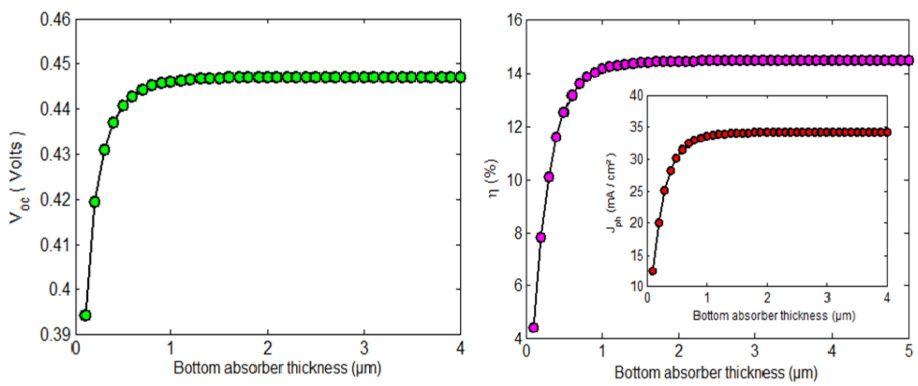

Figure 2: CZTSe solar cell performance as function of absorber thickness.

It was observed that photocurrent density J_{ph} , open circuit voltage V_{oc} and efficiency were found increasing with the CZTSe absorber thickness increase in the range 0.1 to 2 µm. Above 2 µm, the results are saturated.

An optimal thickness of 2 µm was then considered for which a maximum efficiency of 14.46 % was reached with J_{ph} = 34.18 mA/cm² and V_{oc}= 0.4472 V.

The photocurrent density of the tandem cell is limited by the lowest one produced by the sub-cells. Therefore, the current matched condition should be achieved.

The current matching analyze depicted in Figure 3 was carried out by fixing the CZTSe bottom cell absorber thickness at the optimized 2µm value above mentioned and varying the CZTS top cell absorber thickness. The intersection of the obtained curves reveals the current density for both cells matches with a value of 16.54 mA /cm² for a top cell absorber thickness of about 414 nm.

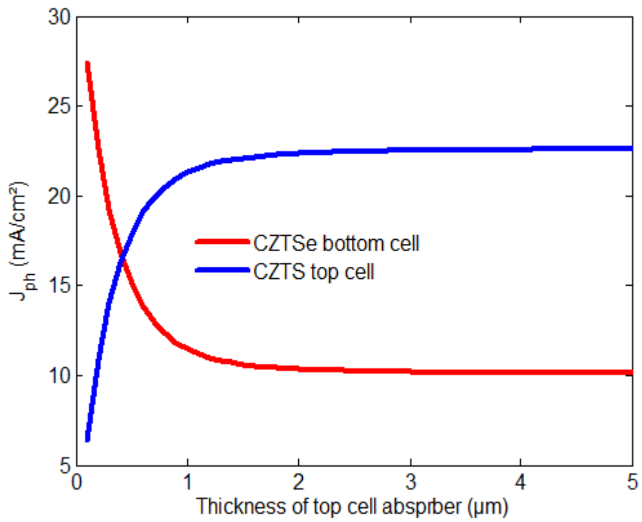

Figure 3: Photocurrent density as function of top cell absorber thickness.

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

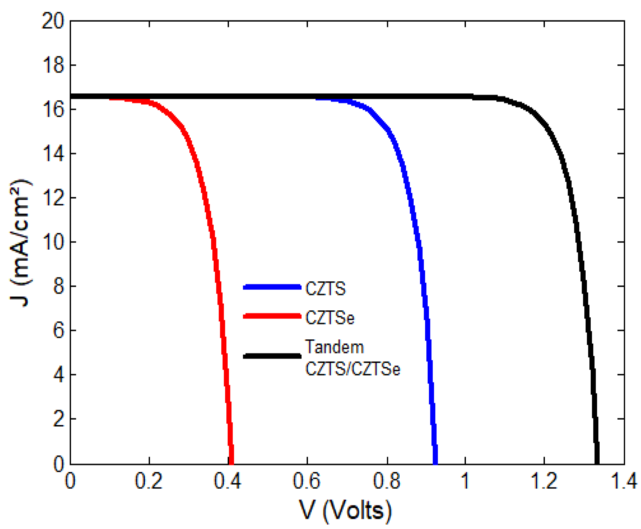

Figure 4 : J(V) characteristics of top, bottom and tandem solar cells.

The advantage of the tandem structure appears in term of improved open circuit voltage, which is the sum of their of top and bottom cells.

The optimized thicknesses of CZTSe bottom and CZTS top cell absorbers yield to a 24.68 % efficiency with 1.33 V open circuit voltage, 16.56 mA/cm² short circuit current density and 78.2% fill factor.

In order to improve the performance of the tandem cell, light trapping techniques are usually used in order to increase the absorption in the device.

Adding a back mirror in the bottom cell leads to a double pass absorption in the CZTSe absorber and improves the bottom cell efficiency and consequently the tandem device efficiency rises to 24.8%.

The effect of randomly textured top cell absorber on performance device was simulated in this paper. The absorptivity of both top and bottom cells was calculated by equations (5) and (6).

The thickness of the CZTS top absorber was also determined according to the current match condition.

The results showed that current densities of top and bottom cells matches at the a reduced top CZTS absorber thickness of 269.8 nm at which 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.

To close this study, the effect of using ZnS instead CdS buffer material in both sub-cells was investigated. The simulation results have showed that the optimal thickness of CZTSe bottom absorber can be reduced to 1.5 µm when ZnS buffer material is used. The photocurrent density variation of both sub-cells against top absorber thickness has showed that the density of current value matches with 16.67 mA/cm² for both top and bottom cells, when the thickness of CZTS top absorber is about 41 nm.

The current density- voltage characteristic of the ZnS buffered tandem solar cell was compared to that of CdS buffer. The curves are represented in Figure 5 .

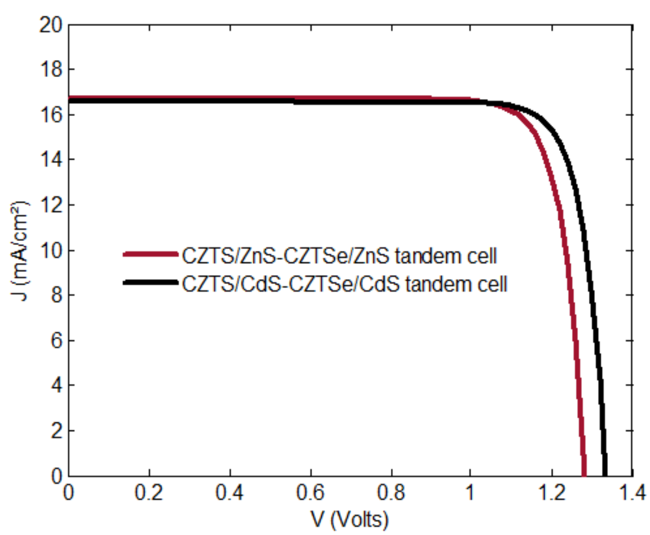

Figure 5: J(V) characteristic of ZnS buffered CZTS/CZTSe tandem cell.

The CZTS/CZTSe tandem solar cell based on ZnS buffers material yield to a 23.83 % efficiency with 1.28 V open circuit voltage, 16.67 mA/cm² short circuit current density and 78% fill factor.

5 Conclusion

In this study, a tandem solar cell based on kestrite CZTS and CZTSe absorbers has been investigated. An optimal thickness of CZTSe bottom cell absorber of 2 µm has been considered, while the CZTS top cell absorber has been adjusted in order to achieve the current matched condition. The simulation results showed that both top and bottom cells matches with a photocurrent density value of 16.54 mA / cm² when top cell CZTS absorber thickness is 414 nm. An efficiency of 24.7 % was achieved with an open circuit voltage of 1.33 V and a fill factor of 78.2%.

Light trapping techniques were studied in this work. It has been found that the use of a back mirror in the bottom cell contributes to achieving an efficiency of 24.8%. However, the use of randomly textured CZTS top cell absorber surface allowed the reduction of its thickness to 270 nm while maintaining the same efficiency of 24.7% with V_{oc} = 1.33 V and J_{ph} = 16, 56 mA / cm².

Finally, using ZnS buffer instead toxic CdS in both sub-cells was investigated. The results of the simulation have shown that the thickness of CZTSe can be reduced to the optimal value of 1.5 µm while that of CZTS at which both sub-cells photo current density matches is 410 nm. An efficiency of 23.83% was obtained with V_{oc} = 1.28 V , J_{ph} = 16, 67 mA / cm², and FF = 78%

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