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Thickness optimization of the ZnO based TCO layer in a CZTSSe solar cell. Evolution of its performance with thickness when external temperature changes.

Meriem Chadel^{1,2,3,a)}, Mohammed Moustafa Bouzaki^{1,2,3}, Asma Chadel¹,
Michel Aillerie^{2,3,b)}, and Boumediene Benyoucef¹

¹University of Tlemcen, URMER, 13000 Tlemcen, Algeria.

²Université de Lorraine, LMOPS, EA 4423, 57070 Metz, France.

³Centrale Supélec, LMOPS, 57070 Metz, France.

E-mail: ^{a)} ch_meriem_ph@yahoo.fr ^{b)} aillerie@metz.supelec.fr

Abstract. The influence of the thickness of a Zinc Oxide (ZnO) transparent conductive oxide (TCO) layer on the performance of the CZTSSe solar cell is shown in detail. In a photovoltaic cell, the thickness of each layer largely influence the performance of the solar cell and optimization of each layer constitutes a complete work. Here, using the Solar Cell Capacitance Simulation (SCAPS) software, we present simulation results obtained in the analyze of the influence of the TCO layer thickness on the performance of a CZTSSe solar cell, starting from performance of a CZTSSe solar cell commercialized in 2014 with an initial efficiency equal to 12.6%. In simulation, the temperature was considered as a functioning parameter and the evolution of the performance of the cell for various thickness of the TCO layer when the external temperature changes is simulated and discussed. The best efficiency of the solar cell based in CZTSSe is obtained with a ZnO thickness equal to 50 nm and low temperature. Based on the considered marketed cell, we show a technological possible increase of the global efficiency achieving 13% by optimization of ZnO based TCO layer.

1. Introduction

Solar cells based on an absorber layer of $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$ (CZTSSe) are considered as a promising photovoltaic device [1] for low cost [2] and high efficiency thin film solar cells. CZTSSe possesses an optimum optical band gap energy between 1.0 and 1.5 eV [3, 4], a high absorption coefficient higher than 10^4cm^{-1} [5, 6]. It consists of earth abundant elements and also considered as an alternative to the expensive and toxic $\text{CuIn}_{1-x}\text{Ga}_x(\text{S}_y, \text{Se}_{1-y})_2$ (CIGSSe) and CdTe currently used as thin film solar cells [7, 8]. Watson, in 2013 obtained the best performances for CZTSSe based solar cells with power conversion efficiency equal to 12.6% [8, 9]. Several research groups reported the growth and fabrication of CZTSSe solar cells using various methods such as sputtering followed sulfo-selenization [10, 11], solution growth process [12, 13], nano-particle approach [14, 15], electrodeposition [16, 17], ink jet printing [18], pulsed laser deposition [19, 20], ball milling and hybrid ink followed by sulfo-selenization [21, 22].

In the reference cell [8], the absorber layer CZTSSe was deposit on a Mo/glass-substrate followed by a Cadmium Sulfide (CdS) buffer layer and a ZnO transparent conducting oxide layer. CdS material



with the energy gap of 2.4 eV is used for the buffer layer in numerous photovoltaic cells [1-2, 7-9]. Experimental details of the cell fabrication are given in Refs. [1, 3, 8]. In the reference cell, the widths of the various layers are as follows: ZnO (200nm)/ CdS (50 nm)/ CZTSSe (2 μ m)/Mo/glass-substrate. Thicknesses of all layers play individually, but also collectively important role in the global efficiency of the cell. For this purpose, in the current contribution, we analyze by simulation the influence of the TCO thickness on the performance of the cell considering, for a clear analysis, constant the parameters of the other layers. This simulation is performed by using the Solar Cell Capacitance Simulation (SCAPS) simulator.

Within the same procedure we analyze the influence of the temperature on the performance of the CZTSSe solar cell considering the optimized structure found by simulation with the ZnO based transparent conductive oxide (TCO) layer, and by comparison with the reference cell, we discuss the influence of the thickness of this layer on the performance of the cell when the temperature change.

2. The reference solar cell

The structure of the reference CZTSSe solar cell is represented in Figure 1. It is designed with the CZTSSe absorber layer deposited on a Mo/glass-substrate. On this layer, with respect of the lattice parameters, a CdS buffer layer was grown and followed by a deposition of ZnO transparent conductive oxide layer. On the top surface of the TCO layer, metal flat bands assume the electrical contacts.

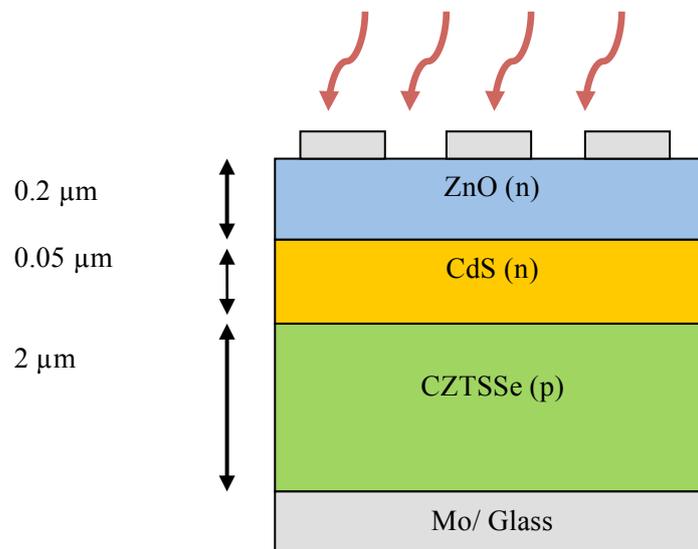


Figure 1. Structure of the simulated solar cell based in CZTSSe.

The band gap of the CZTSSe depends of the ratio S/Se in the material and can vary from 1 to 1.5 eV. In CZTSSe solar cell, the band gap (E_g) of the absorber layer is generally chosen equal to 1.13 eV [23, 24]. For each layer, all useful material parameters were introduced in the simulator code. In addition, Closely to the reference structure, in this simulation, we have introduced flat bands as front contacts, for which SCAPS software automatically calculates the metal work function depending upon whether it is n-type or p-type or intrinsic type layers [25-26]. For the flat band calculations, the layer adjacent to the contact was considered.

The necessary parameters of the materials for each layers in the reference solar cell are the thicknesses for each layer, as mentioned in figure 1 and, additionally to the above mentioned values for the energy gaps $E_{g-CZTSSe}=1.13$ eV for the CZTSSe layer, $E_{g-CdS}=2.4$ eV for the CdS layer, and $E_{g-ZnO}=3.37$ eV for the ZnO based TCO layer. We note that the necessary parameters, used in this contribution were taken from literature values [8, 27, 28].

The external parameters considered as fixed for this simulation are the solar spectrum, equal to AM.1.5, the series resistance (R_s), $R_s=0.36 \Omega.cm^2$ and the shunt resistance (R_{sh}) $R_{sh}=1000 \Omega.cm^2$.

As far as we are concerned, namely the ZnO layer, we recall that this material is no toxic material, low cost, and presents a high stability [29, 30].

Before starting the performance analysis of our structure, we validate our model for the commercial cell [8] with the simulator SCAPS. The result of this first study is illustrated in figure 2 by the current density-voltage (J - V) characteristic for the reference CZTSSe solar cell.

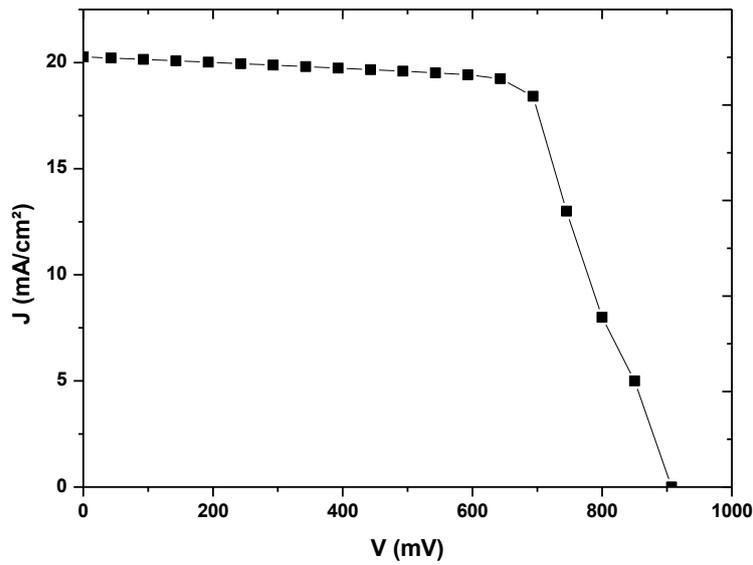


Figure 2. J - V Characteristics of the reference solar cell.

The efficiency of CdS/CZTSSe solar cell is 12.75%, which is not very different from that of a practical solar cell CZTSSe obtained by W. Wang et al and equal to 12.6% in ref [8]. This shows that our solar cell model is valid and accurate, with an error gap compare to practical values less than 1.2% and that it can be used to study the effects of the ZnO based TCO layer thickness on the performance of the cell.

3. Optimization of the TCO layer thickness

Figure 3 shows the evolution of the performance parameters of the cell, i.e. the short-circuit current density (J_{SC}), open-circuit voltage (V_{OC}), fill factor (FF), and efficiency (η) of the CZTSSe solar cell as a function of the thickness ZnO based TCO layer from 0.05 μm to 0.2 μm . These two considered values for the thickness of the TCO layer in our simulation are industrially possible for commercial cells.

The open circuit voltage is relatively constant with the thickness of the ZnO layer. On the contrary, J_{SC} decreases from the 20.68 mA/cm^2 to 20.27 mA/cm^2 when the thickness of the ZnO layer increased from 0.05 μm to 0.2 μm . In Ref. [31] Gordon shows that the increase of the TCO thickness directly induces an increase of the optical absorption in the layer of the incident light at the front side of the cell. This optical absorption is linked to the internal scattering inducing a longer light path-length proportional to the thickness. Thus this loss in the TCO layer due to absorption decreases the amount of photons taking part in the photo-electronic conversion process in the active layers of the cell, with a direct consequence of the decrease of the current and of course, its short circuit value J_{SC} .

By cons, we observe that the FF is only slightly improved starting at 69% for a layer with a thickness equal to 0.05 μm growing close 69.5% for that having a thickness equal to 0.2 μm . in fact,

the main photovoltaic process takes place in the buffer and absorber layers and the form of the J-V characteristic is not significantly changed by a change of the thickness of the TCO layer.

Finally, we can see the huge influence of the thickness of the TCO layer on the efficiency of the cell, which is the highest, equal to 13% for the thinnest TCO layer, and after a continuous decrease with the thickness when the layer possesses the thickness of the reference cell, i.e. down to an efficiency equal to 12.75% for a thickness equal to 0.2 μm . This loss of efficiency is straightforwardly linked to the decrease of the number of photons crossing through the TCO layer with the thickness, i.e. the decrease of the current density participating in the photovoltaic process, as explained above. Thus, the transparent conductive layer thickness increases deteriorates the cell performances.

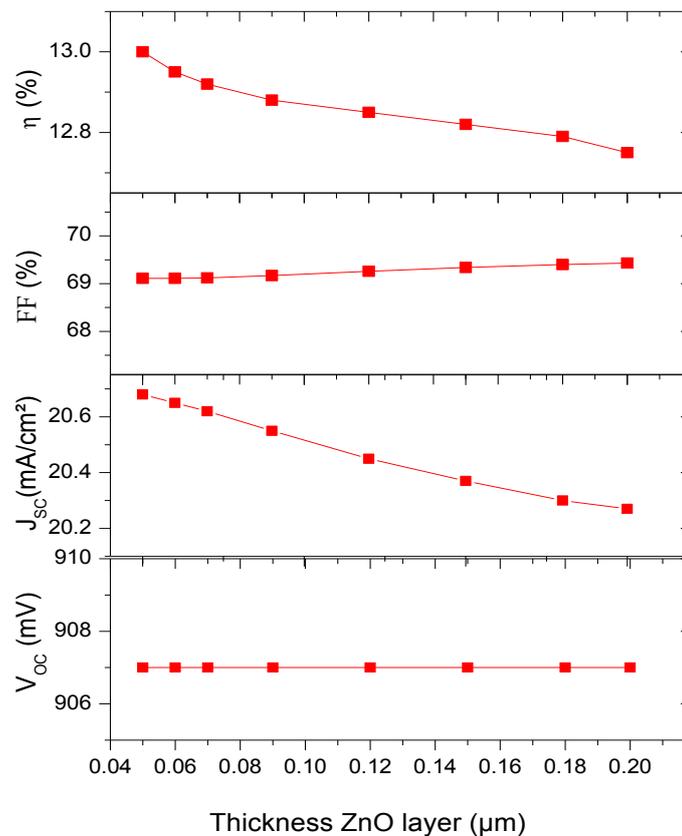


Figure 3. Effects of the thickness of the TCO layer on the performance of the CZTSSe solar cell.

Now, the relative questions to the above simulation results concern the knowledge of the performance of the optimization cell with a change of temperature and if the integration of a thinner TCO layer presents significant advantages in term of efficiency over the entire operating temperature range.

4. Influence of the temperature on the performance of the optimized solar cell

In this section, we consider the same performance parameters for the cell than those considered above except the thickness of the ZnO based TCO layer. In this paragraph, simulations were done with two different thicknesses of the TCO layer, one corresponding to that of the reference cell, i.e. a thickness equal to 0.2 μm and the second to the optimized one, i.e. a thickness equal to 0.05 μm . We have plotted in Figure 4, the evolution of the performance parameters of the CZTSSe solar cell in the temperature range from 5°C to 70°C, corresponding to the generally considered temperature range in practical functioning conditions for both structures.

It is clear from the curves in Figure 4 that J_{SC} slightly increases with increasing temperature with a higher current in all the temperature range for the cell having the thinner TCO layer compared to the reference cell as already mentioned and explained in the previous paragraph. According to the well-known Varshni relationship for temperature dependence of the bandgap energy, this slight increase of J_{SC} reveals small bandgap shrinkage with temperature of the CZTSSe cell. The decrease of E_g with temperature results of a higher absorption for incident light at visible and IR wavelengths inducing an increase of J_{SC} .

By cons, V_{OC} largely decreases when the temperature increase but no difference occurs in both reference and optimized cells confirming the same V_{OC} observed above for cells having various TCO thicknesses in the all temperature range.

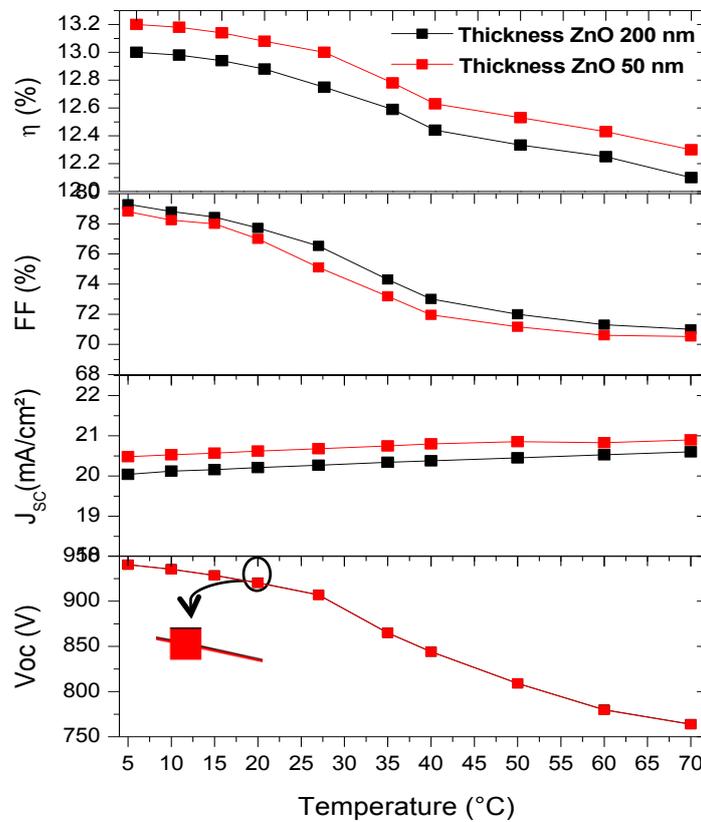


Figure 4. The performance of the CZTSSe solar cell as function of temperature for two thicknesses of the cell.

In Ref. [32], Cai et al. have modeled the dependence of V_{OC} with the temperature for CZTSSe cells. Thus, the relation they suggested between V_{OC} and the temperature can be written as [32]:

$$\frac{dV_{OC}}{dT} = - \frac{V_{g0} - V_{OC} + \frac{\gamma kT}{q}}{T} \tag{1}$$

where V_{g0} is the equivalent voltage of the semiconductor band gap at absolute zero temperature (T) obtained by linear extrapolation; γ includes temperature related factors determining the reverse saturation current density; q is the electronic charge and is equal to 1.6×10^{-19} eV and k is the Boltzman constant.

Thus, Eq. 1 shows that V_{OC} is independent of the TCO thickness and is only linked to the thermal agitation of the charge carriers being important at the atomic level. Indeed, an increase of the electronic vibration leads to an increase of the recombination rate, and thus, a decrease in the voltage values of the solar cell with temperature.

We also show in Figure 4 that the evolution of FF and η with temperature present same behavior that V_{OC} . It is due to the fact that FF is a function of V_{OC} and presents the same change with temperature and, thus, also decreases when temperature increase. In fact, FF depends of other functional parameters of the cell but results of simulation prove that, even if other factors as J_{SC} increase with temperature, the decrease of V_{OC} plays a more important role in FF, which finally decreases with temperature. In the same way, as already well known in solar cell performances, the efficiency of the solar cell decreases with the temperature.

In our simulation we observe that the gap in the efficiency between both reference and optimized cells is found equal to around 0.25%. This difference remains quasi-constant in the whole temperature range, with an absolute decrease for both cell of around 8% for a change of temperature equal to 65° temperature range (from 5°C to 70°C).

5. Conclusion

In this contribution, we have studied the thickness of the ZnO based TCO layer as a parameter to be optimized in order to improve the performances of a CZTSSe solar cell. We have considered the range of the TCO layer thickness by the technologically feasible thickness in commercial cells. From the results of simulation obtained with SCAPS software on the basis of a commercial CZTSSe solar cell, we have shown that the performances of a CZTSSe solar cell can be improved by the decrease of the thickness of its TCO layer. Thus, in our study, the best performances of the solar cell based on CZTSSe, compared with those of a reference cell, are obtained with a cell having a thickness of 50 nm of the ZnO based TCO layer whatever is the considered temperature in the 5-70° range. This thickness remains a technological possible solution for commercial cells.

Finally, we found that the decrease of the efficiency is equal to 8%, passing from 13.2% to 12.2% for a change of temperature equal to 65° (from 5°C to 70°C). It results at room temperature, for the optimized cell having a ZnO based TCO layer equal to 0.05 μm , an efficiency equal to 13%, a fill factor equal to 69.1%, a current density of short circuit equal to 20.68 mA/cm^2 and an open circuit of voltage equal to 907 mV.

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