Enhancement of Output Parameters of Cu_2ZnSnS_4 (CZTS)-based Solar Cells: Numerical simulation using AMPS-1D and SCAPS-1D programs

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Abstract

The presence of impurities in Cu_2ZnSnS_4 (CZTS) thin film material is harmful on output performance of fabricated solar cells. Moreover, the formation of unstable and high resistance contacts to CZTS can contribute to lowering of the thin film solar cells efficiency value. In this study, the performance of the baseline ZnO/CdS/CZTS cell structure is numerically evaluated using AMPS-1D and SCAPS-1D programs. The effect of back contact material, acceptor concentration as well as the absorber thickness on CZTS cell performance was done by AMPS-1D program, whereas the influences of the gap energy of the absorber layer and the operating temperature on cell performance was simulated by SCAPS-1D program. The simulation result revealed that it is not necessary to use a thicker absorber if we want to make a tradeoff between the cell efficiency and the cost for a mass production. It is also important to control and to limit the carrier density in the absorber for efficient CZTS solar cells. The influence of operating temperature on cell performance showed that an increase in the temperature will strongly affect the performance of the cell. The presented work is essential because it can contribute to full understanding of the performance of CZTS solar cell and to the fabrication of cells with a precise control of the process parameters.

1. Introduction

Recently, the renewable energy sector has continued to drive in the mind of researchers a major interest. In particular, photovoltaic (PV) technology continues to grow thanks to the development of new fabrication techniques and the improvement of the solar cells conversion efficiency. Nowadays, the solar cell market is still dominated by wafer-based silicon technology. Due to the indirect band gap of Si, the typical thickness of the cells is about 200 μm [1, 2]. That means large quantity of high quality materials is needed because of the long paths that the photo-generated carriers must travel leading to significant increase in the total cost of the module. Making simple and low cost production processes for fabricated solar cells which use less material could reduce considerably their costs. This could be possible by developing thin film solar cells because this technology uses less material. A number of alternative materials have been investigated for the development of next generation of cost-effective and high efficiency solar cells. Among them Copper Indium Gallium Diselenide (CIGS) [3-5] and Cadmium Telluride (CdTe) [6,7] have shown high efficiencies of 20.3% and 16.5% respectively and have already reached the stage of commercialization [8-11]. However, the scarcity and the toxicity of materials such as Indium, Telluride, Cadmium and Selenium could be a difficult problem for the development of thin film solar cells based on these materials. Developing new PV materials, which are cost-effective and composed of non-toxic and abundant elements in the earth's crust could therefore be a good way to overcome to overcome these issues. Recently, a broad interest has been given to the CZTS material due to its excellent semiconductor properties such as a direct and a tunable band gap energy in the range of 1.4-1.6 eV and large absorption coefficient over 10^4 cm^{-1} [12, 13]. Moreover, all its elements are non-toxic and still available in the Earth's crust [14]. Various physical and chemical techniques have been investigated to fabricate CZTS thin film, namely co-sputtering [15], thermal evaporation [16], pulse laser deposition [17], sol-gel method [18], electrodeposition [19], etc. The conversion efficiency of CZTS-based solar cells has been improved from 0.66% in 1996 to 12.6% in 2014 [18, 20]. Despite the development of different techniques and the improvement of conversion efficiency, our comprehension of this type of solar cell is still relatively limited compared to other solar cells, like silicon-, CdTe- and CIGS-based solar cells. In order to fully understand the performance of CZTS thin film solar cell and to fabricate cells with higher efficiency, a complete investigation of the operation mechanisms of CZTS solar cell is necessary. An approach to reach this goal is to use numerical simulation because it enables researchers to perform theoretical studies on the overall characteristics and performance of solar cells. Although we can observe generally marginal differences between the efficiency of a fabricated solar cell and the one of a simulated solar cell, which is mainly due to the complexity of fabrication process and which may induce many other physical electronic processes that numerical simulation cannot replicate or take into account, it offers however a great opportunity to the scientific community to understand and explore the working principles of various photovoltaic devices prior to the practical cell fabrication and characterization.

In this report, we have evaluated the performances of CZTS-based solar cells by means of numerical simulations. The effect of back metal contact work function, acceptor concentration, absorber thickness on the overall performances of the cell is investigated by the AMPS-1D program and the influence of the gap energy of the absorber layer and the operating temperature on cell performance was simulated by SCAPS-1D program. The details of structure and simulation of the device are stated in following sections.

1. Improvement of CZTS-based solar cells performance using AMPS-1D

In this section, we have studied the effect of back metal contact work function, acceptor concentration, absorber thickness on the output parameters of the CZTS-based solar cells.

1.1 Device structure and simulation

In this study, numerical modeling of CZTS thin film solar cell has been carried out by AMPS-1D program. The computer simulation software AMPS-1D (Analysis of Microelectronic and Photonic Structures) [21] was employed by specifying the semiconductor parameters in each defined layer of the cell structure as input parameters to the simulation. Developed by the Stephen Fonash's group at the Pennsylvania State University in USA, the uniqueness of this software is its ability to examine a variety of device structures such as: [22] homo-junction and hetero-junction p-n and p-i-n solar cells and detectors, multi-junction solar cell structures, novel photovoltaic and optoelectronic structures, Schottky barrier devices with optional back layers [22, 23]. In addition, it evaluates the recombination profile, band diagram under steady-state and carrier transport in one dimension based on the Poisson's equation, the continuity equation for free electrons and the continuity equation for free holes given respectively by [22]:

$$\frac{d}{dx}\left(-\varepsilon(x)\frac{d\psi}{dx}\right) = q[p(x) - n(x) + N_D^+(x) - N_A^-(x) + p_t(x) - n_t(x)] \tag{1}$$

$$\frac{1}{q}\left(\frac{d}{dx}J_n\right) = -G_{op}(x) + R(x) \tag{2}$$

$$\frac{1}{q}\left(\frac{d}{dx}J_p\right) = G_{op}(x) + R(x) \tag{3}$$

where the electrostatic potential ψ, the free electron n and free hole p, trapped electron n_t and trapped hole p_t as well as ionized donor-like doping N_D^+ and ionized acceptor-like doping N_A^- concentrations are all given in terms of the different band gap energy levels by the Boltzmann and Fermi-Dirac distributions, and are a function of the position "x". J_n and J_p are the electron and hole current densities respectively. The term G_{op} is the optical carrier generation rate due to illumination and R is the total recombination rate accounting for direct (band to band) and indirect (Shockley-Read-Hall) recombination traffics.

The CZTS solar cell structure used in this simulation consists of the following layers: ZnO window layer, CdS buffer, CZTS absorber and Mo back contact metal on glass substrate. Figure 1 illustrates the vertical cross section of the typical cell. The device is considered to be illuminated from the front ZnO to the end of the device with the AM1.5 spectrum. Outputs such as current-voltage characteristics under dark and under illumination, the quantum efficiency, the reflectivity and internal quantities such as the electric field, the free and trapped carrier concentrations, the electron and hole currents, the recombination and generation rates can be extracted from the solutions provided by an AMPS simulation. The basic input parameters used in this simulation were selected based on literature, theory and in some cases reasonably estimated and are specific to the device and materials properties. The front contact is considered as a standard ohmic contact and the back contact is choosing for optimizing the cell performance. The basic input parameters used in this simulation are shown in Table 1. The front surface reflectivity and the back surface reflectivity are set to 0.1 and 0.8 respectively in order to reflect experimental quantum efficiency data. The default illumination temperature is set to 300 K and the default illumination spectrum is set to the global standard AM 1.5.

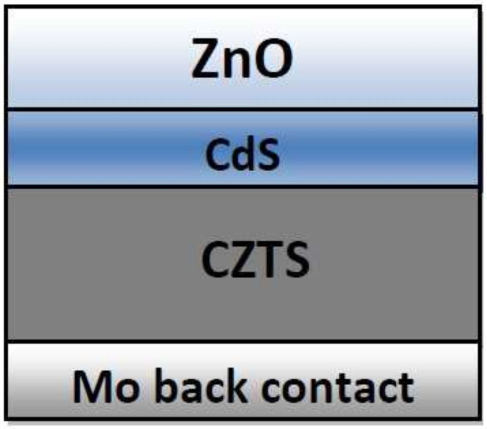

Figure 1. Typical CZTS solar cell structure

Table 1. Main material properties used in the simulation

Material	**window** *ZnO*	**buffer** *CdS*	**absorber** *CZTS*
Energy band gap Eg (eV)	3.30	2.40	1.50
Thickness (nm)	200	60	2000
Donor concentration N_D (cm^{-3})	$1x10^{18}$	$1x10^{18}$	0
Acceptor concentration N_A (cm^{-3})	0	0	$4x10^{16}$
Electron Mobility MUN (Cm^2/Vs)	100	100	100
Hole Mobility MUP (Cm^2/Vs)	25	25	25
Relative permittivity EPS	9	10	10
Effective density of states Nc (Cm^{-3})	$2.2x10^{19}$	$2.2x10^{18}$	$2.2x10^{18}$
Effective density of states Nv (Cm^{-3})	$1.8x10^{19}$	$1.8x10^{19}$	$1.8x10^{18}$
Electron affinity CHI (eV)	4.40	3.80	4.10
Gaussian defect N_G (Cm^{-3})	$1x10^{17}$	$1x10^{18}$	$2.61x10^{15}$

1.2 Results and discussion

Figure 2 below shows the simulated J-V characteristics of the CZTS thin film solar cell obtained with the data of Table 1. The results of our simulation were in good agreement with reported experimental results of the first Mo/CZTS/CdS/ZnO solar cell (J_{SC}=13 mA/cm; V_{OC}=0.541 V; FF=59.8%; η=4.1%) [24]. Parameters like open circuit voltage (Voc), quantum efficiency and series resistances (Rs) are the three fundamental factors which limit the performance of CZTS solar cell [25]. The short current density (Jsc) of the solar cell is affected by the electron transport properties at the ZnO/CdS interface and also by shading losses caused by the front metal contact on the top of ZnO layer. Normally, 11% area of PV cell front surface is occupied by metallic contacts for charge carriers' collection and this can limit the Jsc, induce series resistive components which deteriorate the carrier collection efficiency and therefore the performance [25]. This aspect must be well controlled in order to improve the performance of solar cells.

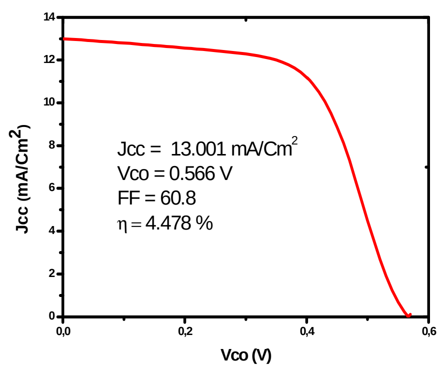

Figure 2.Simulated J-V characteristics of the traditional Mo/CZTS/CdS/ZnO solar cell

A. Effect of back metal work function

To evaluate the effect of the electron work function of the back metallic contact, its value was varied from 5 to 6 eV in this simulation. There is an incredible improvement in solar cell parameters when increasing the electron work function of the back metal contact as shown in Figure 3. One can see in Figure 3 that the efficiency increases considerably as the back metal work function increases from 5.0 to 5.6 eV, which is due to the increase in Jsc, Voc and FF values. As the back metal work function increases, the Schottky barrier created at the back increases and prevents strong recombination of free charge carriers.

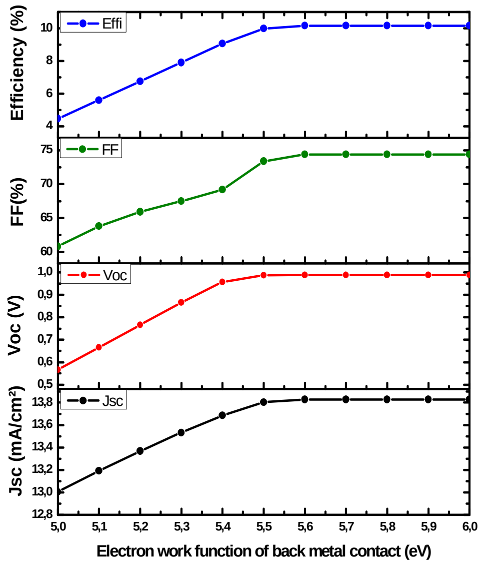

Figure 3. Simulated normalized output parameters of the CZTS solar cell as a function of back metal work function

This effect can improve the value of Voc and therefore the efficiency. No changes in values of Jsc, Voc and FF is observed for back metal work function value between 5.6 and 6 eV and this cause the efficiency to remain also constant in this range. We can thus choose the value of 5.6 eV as the back metal work function optimum value for achieving CZTS solar cell with good performance as shown by our simulation results.

B. Effect of the CZTS absorber layer's thickness

Thickness is an important parameter for semiconductor devices especially in thin film where the carrier diffusion length is a constraint. In thin film solar cells particularly, a large part of the entire device's thickness is occupied by the absorber layer which plays the role of the active layer. In this layer, photons having energy greater than or equal to the band gap energy of the material are absorbed and are then subjugated to the photovoltaic effect. It is therefore needed to control the absorber layer thickness for achieving the consistent output performance of CZTS solar cells. For that, the effect of CZTS thickness on cell performance of the solar cell is studied in this report by varying the thickness from 800 to 4000 nm. Figure 4 shows the effect of CZTS thin film thickness on the cell performance parameters.

We can notice important improvements in both values of J_{SC} and V_{OC} and hence in the efficiency when the thickness increases to higher values. J_{SC} is improved for CZTS thickness up to 2250 nm and is nearly unchanged after this value. From Figure 4, we can observe individual effect of thickness on the cell performance where the J_{SC} shows a substantial rise compared to V_{OC} which is mostly expected. When the absorber layer is thicker, more photons with longer wavelength are absorbed and as consequence, more electron-hole pairs are generated. Hence more free electrons will be collected at the front and this will increase the J_{SC} and therefore the efficiency. Due to the increase of J_{SC}, the efficiency curve increases following the same evolution as the J_{SC} curve and saturates also above 2250 nm. As optimal value, our simulation indicates that a CZTS thickness up to 2250 nm is sufficient for photons absorption of the AM1.5G radiation due to the high absorption coefficient and direct band gap of CZTS material.

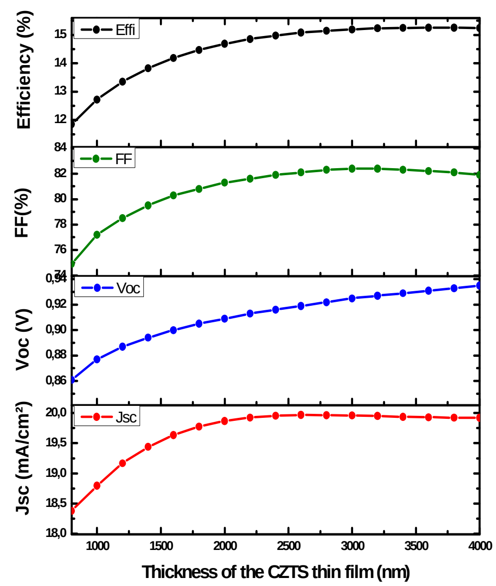

Figure 4. Calculated output parameters of the CZTS solar cell as a function of the thickness

C. Effect of the acceptor concentration in the CZTS absorber

Acceptor defects, characterized with their concentration N_A can be considered as another parameter which limits the solar cell performance. We have varied in our simulation N_A values in the range 10^{13}-10^{18} cm^{-3} in order to evaluate its effect on solar cell performance. We can see on Figure 5 the simulation results of the effect of N_A on output parameters. As carrier concentration increases, the semiconductor material becomes degenerate and this can be harmful for the output performance as shown on Figure 5. In Figure 5, we can see that the J_{SC} decreases with the carrier concentration while the V_{OC} increases with it. The variations in the values of J_{SC} and V_{OC} caused by N_A can be explained by the following simple PN junction model [26].

$$I_0 = Aqn^2\left(\frac{D_e}{L_eN_A}+\frac{D_h}{L_hN_D}\right)$$

(4)

$$V_{OC} = \frac{KT}{q}\ln\left(\frac{I_L}{I_0}+1\right) \quad (5)$$

These equations show that the saturation current I_0 will decrease if N_A increases and therefore V_{OC} will increase if I_0 decreases. This is probably due to the recombination process which is enhanced by increasing N_A. This phenomenon reduces the possibility of free electrons to be collected at the front after being generated by incident light and this can result to limit the J_{SC}. A higher content of N_A in the material will also cause a drop in the value of FF since long wavelength photons are absorbed deeply in the material and the electrons created there are more dependent on diffusion effect to be collected effectively.

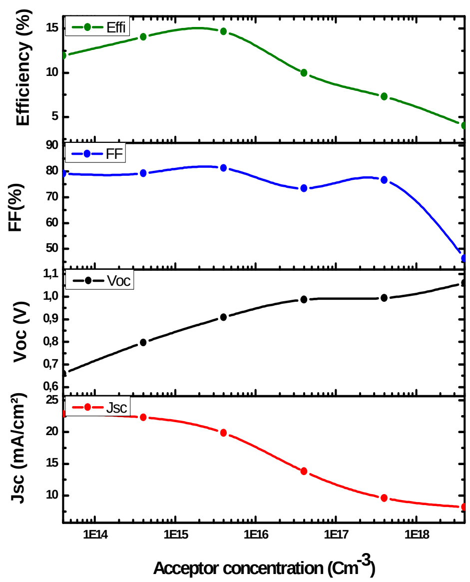

Figure 5. Calculated output parameters of the CZTS solar cell as a function of acceptor concentration

2. Improvement of CZTS-based solar cells performance using SCAPS-1D

In this section, we have investigated the effects of absorber band gap and operating temperature on the overall CZTS solar cell device performance.

1.3 Device structure and simulation

In this study, numerical modeling of CZTS thin film solar cell has been carried out by SCAPS-1D (Solar Cell Capacitance Simulator) version 3.2.00 computer software to investigate the effects of absorber band gap and operating temperature on the overall CZTS solar cell device performance. SCAPS-1D is one-dimensional computer software developed at the University of Ghent under Marc Burgelman [27]. It is developed specially to simulate the AC and DC characteristics of heterojunction thin film solar cells, especially CIGS and CdTe solar cells. One of the special features of SCAPS-1D version 3.2.00 is that it incorporates the defects levels of Gaussian type. Output parameters such as current voltage characteristics in the dark and under illumination can be extracted from a SCAPS simulation. For solar cell and detector structures, collection efficiencies as a function of voltage, light bias, and temperature can also be obtained. In addition, important information such as energy band diagram of the overall cell, occupation probability of deep defects, carrier generation-recombination profiles, individual carrier current densities, electric field distributions, free and trapped carrier populations and recombination profiles as a function of position can be extracted from the SCAPS program. The traditional structure of the solar cell of *Figure 1* was adopted in this study. By incorporating different parameters values of materials in SCAPS software for all aspects of the analysis, one can record the variations of J_{SC}, V_{OC}, FF and efficiency values. The solar cell performance was analyzed from the J-V characteristics.

The basic input parameters used in this simulation which were selected based on literature, theory or in some cases reasonably estimated and specific to the device and materials properties are listed in Table 2 [25, 26]. The default illumination temperature is set to 300 K and the default illumination spectrum is set to the global standard AM 1.5G.

1.4 Results and discussion

The resulting curve of the J-V characteristics of the simulation using values of *Table 2* is shown on *Figure 6* below. The simulated efficiency of our solar cell is 10.27% which is close to the one of a practical solar cell. This result shows that our solar cell model is valid and can be used to investigate the effects of different parameters on overall cell performance.

Table 2 Parameters used in this simulation

Parameters	**ZnO**	**CdS**	**CZTS**
Thickness (μm)	0.2	0.05	2
Energy band gap Eg (eV)	3.35	2.4	1.5
Electron affinity (eV)	4.35	4.0	4.21

Relative permittivity	9	10	10
Effective density of states Nc (Cm^{-3})	$2.2x10^{18}$	$2.2x10^{18}$	$2.2x10^{18}$
Effective density of states Nv (Cm^{-3})	$1.8x10^{19}$	$1.8x10^{19}$	$1.8x10^{19}$
Electron thermal velocity (cm/s)	$1x10^{7}$	$1x10^{7}$	$1x10^{7}$
Hole thermal velocity (cm/s)	$1x10^{7}$	$1x10^{7}$	$1x10^{7}$
Electron Mobility (Cm^2/Vs)	25	25	100
Hole Mobility (Cm^2/Vs)	100	100	20
Donor concentration N_D (cm^{-3})	$1x10^{18}$	$1x10^{18}$	0
Acceptor concentration N_A (cm^{-3})	0	0	$1x10^{16}$
Absorption coefficient	SCAPS	SCAPS	$2.5x10^{4}$

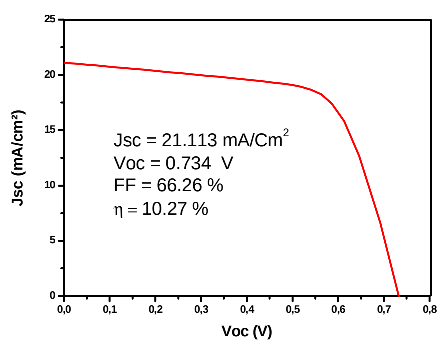

Figure 6. J-V characteristics of the simulated CZTS solar cell

D. Influence of energy band gap on CZTS cell performance

The energy band gap of CZTS absorber layer is varied from 1.1 eV to 1.7 eV by step of 0.1 eV. The performance of the cell is shown in terms of J_{SC}, V_{OC}, FF and efficiency and one can see changes in the values of these parameters as shown in Figure 7. It emerges from Figure 7 that V_{OC} and FF increase substantially up to 1.3 eV and remain almost unchanged after this value while J_{SC} decreases linearly. This decrease can be explained by the fact that absorbers with large energy band gap don't absorb long wavelength photons because they act like a window for these photons. One can note therefore a weak quantity of generated electron-hole pairs and then a weak quantity of collected free charged carriers; and this can reduce the J_{SC} value. The decrease in the efficiency after 1.3 eV is due to the decrease in J_{SC} since V_{OC} and FF are almost constants after this value.

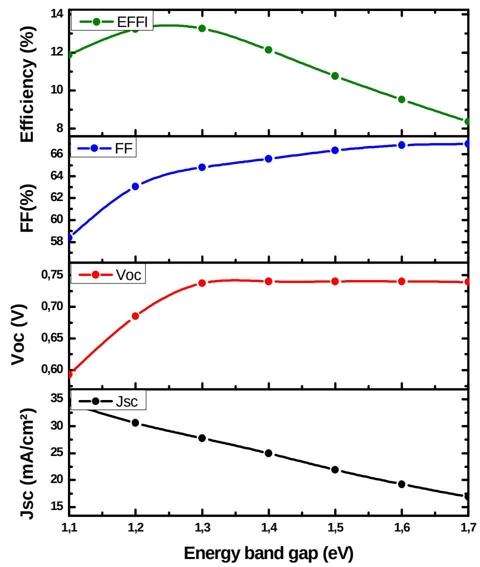

Figure 7. Effect of energy band gap on CZTS cell performance

E. Influence of operating temperature on CZTS cell performance

Since the cell is confronted to different climate conditions, it is important and necessary to investigate the stability of the cell at different operating temperatures. The influences of operating temperature on the output parameters have been studied with the temperature ranged from 280 to 400 K by step of 20 K. As shown in Figure 8, V_{OC}, FF and efficiency are strongly affected by the increase of operating temperature while J_{SC} increases weakly. When the operating temperature increases, electrons in the cell gain additional energies. This causes the electrons to become unstable and more likely to recombine with holes before they reach the depletion region and being collected. This will lead to the decrease of V_{OC} and fill factor. It is important to control all these aspects in order to improve the performances of CZTS-based solar cells.

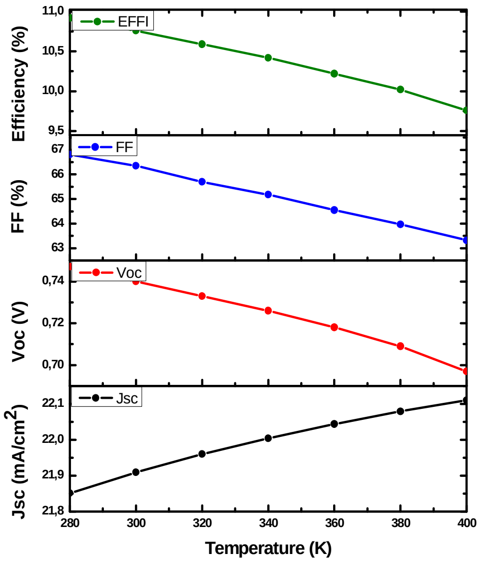

Figure 8. Effect of operating temperature on cell performance

3. Conclusion

In conclusion, a comprehensive study of numerical simulations of CZTS thin film solar cells by AMPS-1D and SCAPS-1D is performed in this report. The simulations results showed that the cell parameters such as CZTS absorber layer thickness, carrier density, defect density, energy band gap have different effects on cell performances. It emerges from simulations that there is a need to fabricate CZTS thin film solar cells by reducing the thickness of CZTS absorber layer as well as with a not so large energy band gap and a limited number of carrier density in the absorber. It is necessary to well control these parameters in order to find a tradeoff between the cell efficiency and its cost for a mass production.

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