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Investigations of achieved performances of solar cells based chalcogenide via TCAD tools

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Abstract

In this work, numerical simulations are performed of both single junction solar cell based copper indium diselenide (CIS) and copper indium gallium diselenide (CIGS) with a window layer (ZnO) and a buffer layer(CdS).The simulation tool used for this study is Silvaco-Atlas package based on the 2D-numerical resolution of the transport equations governing the conduction mechanisms in semiconductor devices. The (J-V) characteristics are simulated under AM1.5G Illumination.

These simulation results show that the cell performance can be achieved by an appropriate choice of optical, physical, electrical and technological parameters characterizing each material of the cell in form of photovoltaic parameters (J_{sc}, η, V_{oc}, FF).

Keywords: SILVACO; ATLAS; CIGS; CIS; TCAD tools.

1. Introduction

The elemental and compound material systems widely used in photovoltaic applications can be produced in a variety of crystalline and non-crystalline forms. Although the crystalline group of materials have exhibited high conversion efficiencies, their production cost are substantially high. Several candidates in the poly- and microcrystalline family of materials have recently gained much attention due to their potential for low cost manufacturability, stability, reliability and good performance, among those materials two options appear clearly in recent years by their performance and simplicity for implementing: the die of CdTe and CuInSe2 (and its variant $Cu(In,Ga)Se_2$ still called CIGS), both as often associated with the CdS window layer [1].

In this work, we have used the Silvaco- Atlas software on the design and the study of two single junction solar cells based copper indium diselenide (CIS) and copper indium gallium diselenide (CIGS). We will show the simulation results of a CdS/CIGS solar cell which exhibits an improvement in the photovoltaic performance compared to the CdS/CIS solar cells.

2. CI(G)S solar cell structure and numerical simulation

The CIS or CIGS cell structure considered in this study consists of the following material layers: n-ZnO (Window), n-CdS (Buffer) and p-CI (G) S (Absorber).

Figure 1 illustrates the different regions of this cell generated by Atlas defining these layers.

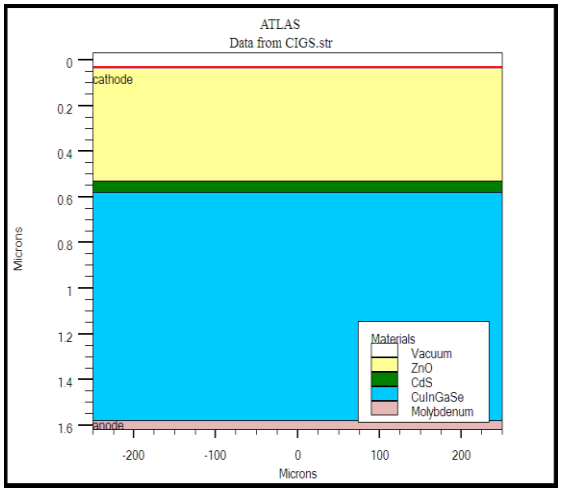

Figure 1. The structure of CI(G)S Solar Cell.

In our simulation the CIS and CIGS solar cells are connected with ZnO layer (transparent conducting oxide layer, TCO). This solar cell was considered illuminated under AM 1.5G solar spectrum with 1000 $W.cm^{-2}$ incident power density [2].

The software Atlas of Silvaco requires the input of the device parameters which are those of material parameters of each layer in the cell structure.

The semiconductor properties of ZnO, CdS, CIS and CIGS layers used as the input parameters for the simulations were given in Table.1, also the doping concentrations of donors and acceptors and thicknesses of these layers.

Table 1. Material parameters used in the simulation

Parameters	ZnO	CdS	CIS/CIGS
Permittivity ε_r (F.cm^{-1})	9	10	13.5
Electron Affinity χ (eV)	4 .5	4.28	4.3
Electron mobility μ_n(cm^2/V.s)	100	350	50
Hole mobility μ_p (cm^2/V.s)	25	50	5
N_A (cm^{-3})	0	0	5.10^{15}
N_D (cm^{-3})	10^{18}	10^{17}	0
Conduction band effective density of states Nc (cm^{-3})	$2.2{\cdot}10^{18}$	$2.2{\cdot}10^{18}$	$2.2{\cdot}10^{18}$
Valence band effective density of states Nv (cm^{-3})	$1.8{\cdot}10^{19}$	$1.8{\cdot}10^{19}$	$1.8{\cdot}10^{19}$
Layer band gap Eg (eV)	3.3	2.4	1.02/1.27
Thickness (nm)	500	50	1000
Gaussian-distributed defect states			
Gaussian defect density D /A (cm^{-3})	10^{17}	10^{16}	10^{15}
Peak energy position (eV)	Eg/2	Eg/2	Eg/2
Standard energy deviation (eV)	0.1	0.1	0.1
Electron capture cross section (cm^2)	10^{-14}	10^{-14}	5.10^{-13}
Hole capture cross section (cm^2)	10^{-15}	10^{-13}	2.10^{-14}

The electron/hole mobility (μ_n and μ_p) of each layer were set according to [2] and [3]. The electron affinity (χ) of CI(G)S was reported to be in the range of 4.10 – 4.90 eV [4] and 4.30eV was chosen for the simulation. The effective density of states of the conduction band (Nc) and of the valence band (Nv), respectively of each layer were set according to [5].

An approximate expression of the band gaps of the semiconductors Cu ($In_{(1-x)}$, Ga_x) Se_2 alloys was used [6].

$$Eg(x) = 1.011 + 0.664x - 0.249(1-x) \quad (1)$$

Where Eg ranging from 1.011 eV to 1.68 eV for x=0 (CIS) and x=1 (CGS), respectively.

The optical parameters of the real and the imaginary parts of the refractive index n(λ) and extinction coefficient k(λ) of the CIS and CIGS materials are obtained from [7] and for ZnO and CdS layers they can be found in [8] and [9]. For metal contact layer (Mo), the optical constants available in the SOPRA database of the Silvaco- Atlas software were used in the simulation. In this study, the solar cells operating temperature was set at 300 K.

Different deposition technologies of this kind of layers have shown a non-crystalline or even polycrystalline structure generating a density of localized defects at the grain boundaries usually modeled by dangling bonds (Gaussian distribution) and single level traps. In our simulation we considered only the dangling bonds because of their proximity to the mid-gap where carrier exchanges are made. The parameters characterizing these defects are reported in Table 1 for the donor and acceptor type for all layers.

Atlas of Silvaco takes into account the Shockley- Read-Hall (SRH) recombination model for these defects to calculate carrier recombination rates [10], [11].

3. Results and discussion

In all the simulation results that will be exposed in the following sections, it is noted that the output parameters are always better in the case of the CIGS than of the CIS in the kind of these thin-film solar cells. This improvement is related to the absorbing layer gap which is 1.27 eV for CIGS and 1.02 eV for CIS, it affects in particular η, Voc and FF against the Jsc is degraded. These results is in good agreement with other work already published [12] even in the case of amorphous silicon solar cells [13].

3.1. Effect of CdS buffer layer thickness

The effect of the CdS layer thickness on both solar cells performances is shown in Figure. 2.

In our simulation, we assume the thickness of the CdS buffer layer was varied from 10 nm to 100 nm when the absorber layer thickness remains constant at 1µm.

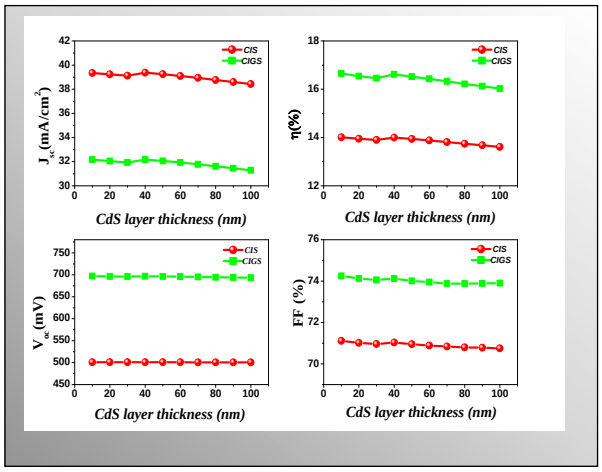

Figure 2. Cell photovoltaic parameters for various buffer layer thicknesses CdS.

It is clear in Figure 2 that CdS layer has no great influence on the performance of both solar cells. Its role is only to create the electric field results of the junction

within of space charge region. So it is preferred that the thickness of the N layer is as small as possible (40 nm in this simulation) to reduce optical absorption losses.

When we increase the thickness of CdS layer, a large number of photons are absorbed in this layer before reaching the absorber layer (CIS or CIGS).

3.2. Effect of CIS or CIGS absorber layer thickness

Figure 3 shows the effect of the thickness of the absorber layer (CIS and CIGS) on the cell performances for the CdS layer thickness fixed at 50 nm. The absorber layer thickness is varied from 0.5 µm to 4 µm.

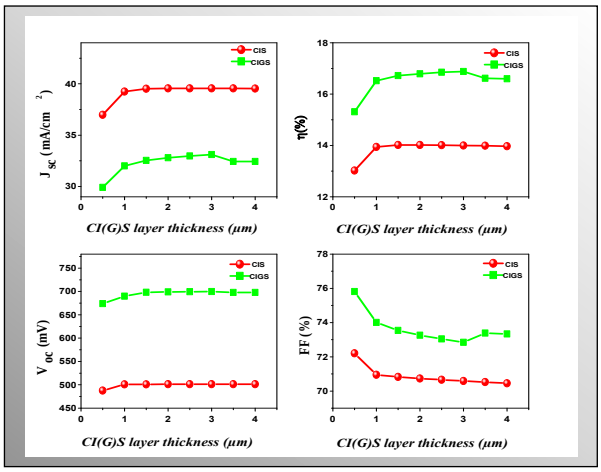

Figure 3. Cell photovoltaic parameters for various absorber layer thicknesses CI(G)S.

It is obvious that the choice of an adequate thickness is important of the absorbing layer for a better conversion of the solar radiation for the wavelengths situated in the visible and the near infrared. In our case, the results of simulations show that the thickness of 1 µm and more is sufficient to maintain the output parameters at an almost constant mean value.

3.3. Effect of CdS doping concentration

The effect of CdS doping concentration on the solar cells performance is shown in Figure. 4 for both absorber layer CIS and CIGS with doping concentration of 5.10^{15} cm^{-3}. The doping concentration of the CdS layer was varied from 10^{15}cm^{-3} to 10^{19}cm^{-3}.

In order to achieve the best performance of any solar cell, it is important to have a high doping concentration of the frontal layer that should be quite thin to minimize the recombination losses of the photo-generated carriers and consequently reach the depletion layer and finally collected. So in this figure, the output parameters show that from a doping-concentration greater than 10^{17}cm^{-3}, the conversion efficiency η and fill factor FF are improved to reach their maximum. However a slight increase is noted for the J_{sc} while the V_{oc} remains almost invariant.

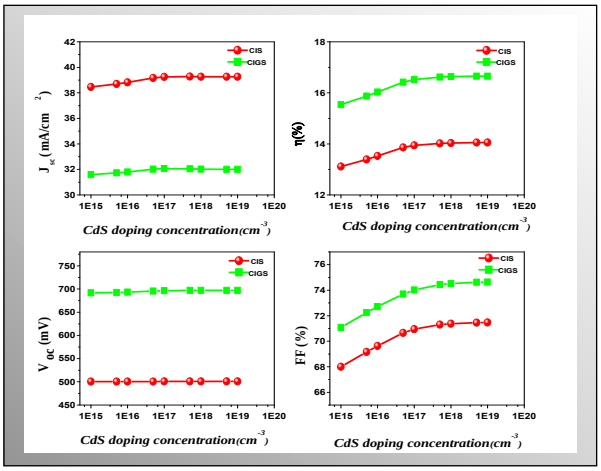

Figure 4. Cell photovoltaic parameters for various buffer layer doping concentration CdS.

We remember that the defects considered in this study are the dangling bonds that have an impact just on the moderately and weakly doped layers because of their location in the mid-gap.

On the other hand, these defects affect the absorber layer that can be seen below.

3.4. Effect of CI(G)S doping concentration

Figure 5 shows the effect of CIS or CIGS doping concentration on the cell performance for CdS layer doping concentration of 10^{17}cm^{-3}. The doping concentration of both absorber layers is varied from 10^{14}cm^{-3} to 10^{17} cm^{-3}. The results of the simulation show that the efficiency reaches its maximum for a doping of 5.10^{15} cm^{-3}. So, it is a value slightly higher than the defects density of states (10^{15} cm^{-3} in Tab. 1) to exhaust the trapping of the photo-generated carriers. The doping concentration must be sufficient to maintain the electric field in the depletion region.

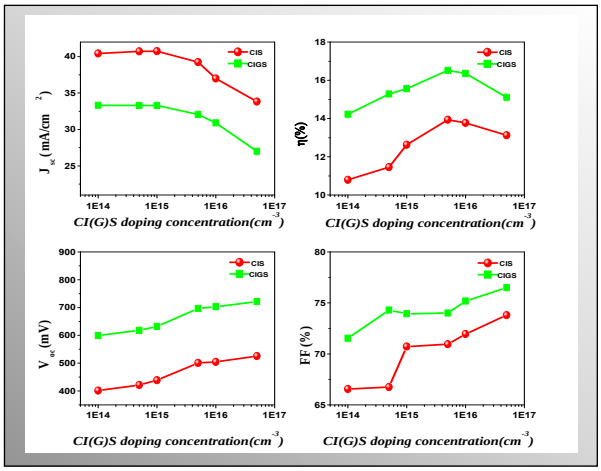

Figure 5. Cell photovoltaic parameters for various absorber layer doping concentration CI(G)S.

4. Conclusion

The results simulation show that by adding the gallium to the CIS absorber layer we boosts its band-gap from its normal 1.02 (eV), which improves the voltage and therefore the efficiency of the device. This particular variation is commonly called a copper indium gallium diselenide or "CIGS" solar cell.

The increases of the buffer layer thickness only reduce the cell performance when the increasing of doping concentration for this later help to improve the collection of generated photo carriers, on the other hand the increasing of the thickness at the absorber layer help to absorb more photons and this would help to produce more electron-hole pairs when the increasing of doping concentration of this same layer imply a difficulty in transport of photo-generated carrier ,So the best output parameters are reached for an CIGS structure with a wide band gap , high concentration doping and thin thickness of CdS window layer, Therefore considering all factors such as doping, thickness of the layer in solar cell junction which can effect and determine the efficiencies of the solar cell. These were investigated in order to obtain the optimum CI(G)S solar cell.

On the other side, due to the toxicity of cadmium many investigations have been done in order to replace CdS by other buffer layer no-toxic [14], [15], [16]. So our future investigation based to replace the CdS buffer layer by other materials no-toxic to obtain a good performance.

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