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Numerical simulation of the effect of varied buffer layers on the performance of Cu(In, Ga)Se2 solar cells using Silvaco Tcad 2D

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The CIGS thin-film solar cells Solar cells are regarded as one of the most promising photovoltaic technologies. They have the advantage of fast and low-cost manufacturing by depositing several thin layers. In this work, a numerical simulation was made to compare the effect of different buffer layers (CdS, ZnS, ZnSe, and In2S3) on the performance of CIGS solar cells using Silvaco Tcad 2D software. The results show that each buffer layer influences the performance of the cell. Therefore, our results suggest that the ZnS material as a buffer layers has better performance for our cell (Jsc=37.0252mAcm2, Voc=1,281, FF=88,01 , η=20,88).

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1. Introduction

Over recent years, thin-film solar cells have attracted attention in the photovoltaic field to produce solar energy. This type of solar cells is preferred because of its low raw material consumption and its lightweight and flexibility. The Cu(In,Ga)Se2 is one of the most promising materials that is quite close to a record number of well-developed conventional silicon technology based on non-flexible wafer material [1]. The CIGS quaternary compound semiconductor is a composition of four materials Copper(Cu), Indium(In), **G**allium (Ga), and Selenium(Se), This compound material has several advantages such as a high optical absorption coefficient (105 cm-1), a variable bandgap of 1,02 EV for CIS up to 1.68 EV for CGS, long-term stability and high theoretical efficiency [2]. A thin-film solar cell-based Cu (In, Ga) Se2 achieve an efficiency of 22.3% by solar Frontier K.K and certified by the Fraunhofer Institute Fur Solare Energysystems (ISE) [3]. A CIGS-based solar cell is composed of several layers of material with the Cu(In,Ga)Se2 as an absorbent layer located between the substrate, the electrical contact and the buffer layer, also known as the window layer. Generally, cadmium sulfide (CdS) is used as a buffer layer. Cds is a II –VI compound semiconductor which has a direct band gap and has the application in optoelectronic devices because of its relatively low electron affinity, high chemical inertness and sputter resistance but due to the environmental pollution resulting from toxic cadmium (Cd), the application of this material in CIGS solar cells has been limited [4,5]. Owing to this problem, solar cell developers are searching for alternative materials. In this paper, we will present a comparative study between the performance (Voc, Jsc, FF, Eff) of a solar cell based CIGS with different buffer layer using the software Silvaco TCAD 2D under standard illumination (AM1.5G, 100w/cm2, 300 k).

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2. Modelling and simulation

We have modeled the J–V characteristics of Cu(In1−x, Gax)Se2 solar cells with the numerical simulation package 2D ATLAS which is a software of Silvaco. This simulator provides general capabilities for physically based two (2D) and three-dimensional (3D) simulation of semiconductor devices. Newton's method is the numerical method used in ATLAS for solving basic semiconductor equations. Poisson’s equations for heterojunction are given by [6]:

$$\frac{d^2\varphi}{dx^2} = -\frac{q}{\varepsilon}(p - n + N_D - N_A) - \frac{1}{\varepsilon}\frac{d\varphi}{dx}\frac{d\varepsilon}{dx} \qquad (1)$$

where q is electron charge, n is electron density, p is hole density, ND is donor impurity density, NA is acceptor impurity density and Ɛ is dielectric constant

$$\frac{\theta n}{\theta t} - \frac{1}{q}\nabla.J_n - U_n = 0 \qquad (2)$$

$$\frac{\theta p}{\theta t} - \frac{1}{q}\nabla.J_p - U_p = 0 \qquad (3)$$

where Jn is electron current density and Jp is hole current density. Un is the generation rate for the electrons and Up is the generation rate for the electrons and holes. The electron and hole currents of heterostructure are given by[7]:

$$J_n = \mu_n n(qE - \frac{d\chi_c}{dx} + \frac{kT}{n}\frac{dn}{dx} - \frac{kT}{N_c}\frac{dN_c}{dx}) \qquad (4)$$

$$J_p = \mu_p p(qE - \frac{d\chi_c}{dx} - \frac{dE_g}{dx} - \frac{kT}{p}\frac{dp}{dx} - \frac{kT}{N_v}\frac{dN_v}{dx}) \qquad (5)$$

Where NC is electron effective density of states and NV is the hole effective density of states.

From equations (4) and (5) we obtain:

$$J_n = -\mu_n q\nabla(V + \theta_n) + kT.\mu_n.\nabla_n \qquad (6)$$

$$J_p = -\mu_p q\nabla(V - \theta_p) + kT.\mu_p.\nabla_p \qquad (7)$$

Where:

$$\theta_n = \frac{\chi_c}{q} - \varphi_0 + \frac{kT}{q}\ln(\frac{N_C}{n_i}) \qquad (8)$$

$$\theta_p = -\frac{1}{q}(\chi_c + E_g) + \varphi_0 + \frac{kT}{q}\ln(\frac{N_v}{n_i}) \qquad (9)$$

Xc is the electron affinity, Eg is the band gap energy, ni is the intrinsic carrier concentration, T is the absolute temperature, k is the Boltzmann's constant, N_C is the conduction band effective density of states, N_V is the valance band effective density of states, φ is the electric potential and φ_0 is reference potential.

The device consists of three layers, the windows layer (ZnO), the buffer layer (CdS, ZnS, ZnSe, InS) and the absorber layer (CIGS). These three layers are identified as ZnO (n-type, $N_D=10^{18}$ Thickness=0.4 μm), buffer layer (n-type, $N_D=10^{17}$, Thickness=0.04 μm), and CIGS (p-type, $N_D=5.10^{16}$, Thickness=3 μm). Fig. 1 shows the structure of the CIGS heterostructure fabricated using a Silvaco TCAD:

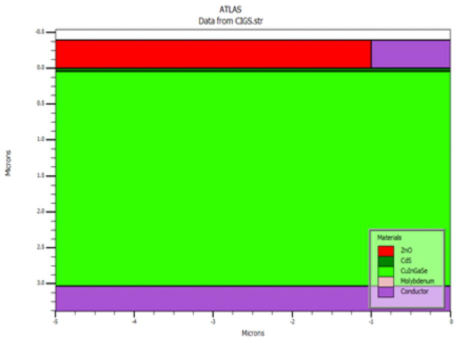

Fig. 1. The structure of CIGS solar cell.

Table 1 show the description for the parameters used in the simulation and the basic parameter that are used in the study [8]:

Table 1. The parameters for the CIGS solar cell at 300K.

Parameters	*ZnO*	*CdS*	*ZnS*	*ZnSe*	*InS*	*CIGS*
Eg(eV)	*3.3*	*2.48*	*3.8*	*2.58*	*2.1*	*1.52*
$\varepsilon_r(F.\ cm^{-1})$	*9*	*10*	*8.3*	*8.01*	*13.5*	*13.6*
$Nc(cm^{-3})$	$2.2\ 10^{18}$	$2.41\ 10^{18}$	$5\ 10^{18}$	$5\ 10^{18}$	$1.8\ 10^{19}$	$2.2\ 10^{18}$
$Nv(cm^{-3})$	$1.8\ 10^{19}$	$2.57\ 10^{19}$	$1.8\ 10^{19}$	$1.8\ 10^{19}$	$4\ 10^{13}$	$1.8\ 10^{19}$
$\chi_e(eV)$	*4*	*4.18*	*4.59*	*4.09*	*4.65*	*4.58*
$\mu_n(cm^2.v^{-1}.\ S^{-1})$	*100*	*100*	*165*	*100*	*400*	*100*
$\mu_p(cm^2.v^{-1}.\ S^{-1})$	*25*	*25*	*5*	*16*	*210*	*25*

3. Results and discussion

In this part, we compare the performances of the solar cell CIGS such as the spectral response characteristics J-V and the maximum power output with different buffer layer using the simulator Silvaco 2D.

3.1. Spectral response simulation

The external quantum efficiency (EQE) is the ratio of the number of carriers collected by the solar cell to the number of incident photons. The curves of external quantum efficiency (EQE) versus wavelength for different buffer layer are shown in Fig. 2:

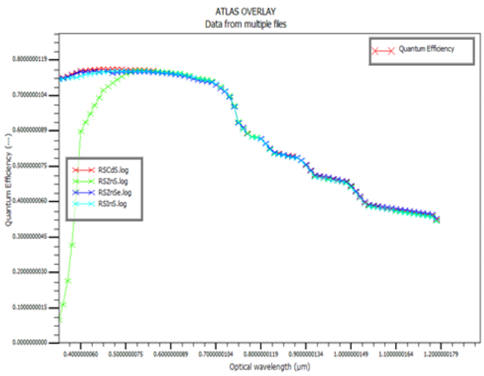

Fig. 2. The spectral response curve for different buffer layer.

We note that EQE curves of these devices in the wavelength region from 350 nm to 1200 nm Solar cells with CdS, ZnSe and InS as buffer layer show higher values of EQE in the short wavelength region (350–500 nm) compared to CIGS based-ZnS buffer layer.

The EQE measurements showed Improved EQE over the whole wavelength for CIGS Solar cell buffered with CdS, ZnS, ZnSe and InS which allowed a higher Jsc.

3.2. Characteristics J-V simulation:

The J-V characteristic of the solar cell Cu(In,Ga)Se with the AM1.5 illumination conditions (100mW/cm2), is shown in Fig. 3 and the main photovoltaic parameters (ISC, VOC, FF and η) are represented in Table 2 for the different buffer layers:

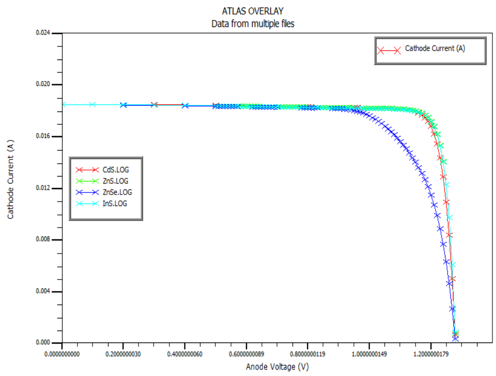

Fig. 3. J-V characteristics for CIGS solar cell with different buffer layer.

From the results obtained, we can remark that ZnS buffer layer based cell has achieved as high efficiency as 20.88%, suggesting it to be a potential replacement of CdS further, InS and ZnSe based buffer layer has achieved efficiencies of 20.81 and 17.68%, respectively. ZnS and InS are very promising as CdS replacement due to higher efficiency than CdS.

Table 2. The photovoltaic parameters for the CIGS solar cell with different buffer layer.

Buffer layer	***Voc (V)***	***Jsc(mA/cm^2)***	***FF(%)***	***η(%)***	***Reference***
CdS(Experimental)	***0.71***	***34.8***	***79.4***	***19.6***	[9]
CdS(Simulated)	***1.28***	***37.02***	***87.25***	***20.69***	***In this work***
ZnS(Experimental)	***0.66***	***36.11***	***78.16***	***18.6***	[10]
ZnS(Simulated)	***1.28***	***37.02***	***88.07***	***20.88***	***In this work***
ZnSe(Experimental)	***0.55***	***34.4***	***73***	***13.6***	[11]
ZnSe(Simulated)	***1.28***	***36.96***	***74.7***	***17.68***	***In this work***
InS(Experimental)	***0.66***	***34.3***	***74.9***	***17.1***	[9]
InS(Simulated)	***1.28***	***37.02***	***87.76***	***20.81***	***In this work***

3.3. Maximum power output

Fig. 4 shows the evolution of the power as a function of the voltage:

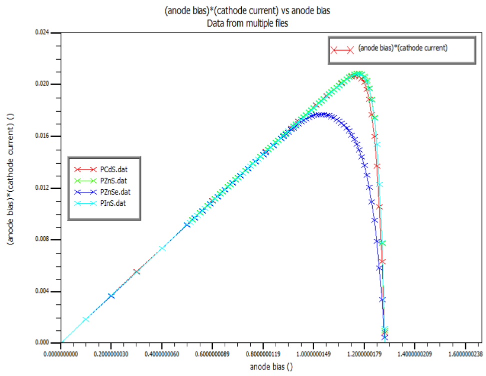

Fig. 4. The maximum power output for CIGS solar cell with different buffer layer.

We notice that more the voltage increases, the power also increases more until reaching the maximum power from which it begins to decrease, the maximum powers of our cell buffered by CdS, ZnS ,ZnSe and InS are 20,69, 20,88, 17,69 and 20,81 respectively[12].

4. Conclusions

In this work, we made a simulation of a solar cell based CIGS using several buffer layers CdS, ZnS, ZnSe and InS. The study consisted of calculating the characteristics of each cell and making comparisons in order to obtain the best structure.

The CdS is to be avoided mainly for these environmental problems however the ZnS and the InS have given higher efficiency than the CdS and the ZnSe gives the lower efficiency.

After the results of our study the best structure is the CIGS/ZnS because of these high photovoltaic parameters (Jsc=37.0252mAcm2, Voc=1,281, FF=88,01 , η=20,88).

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