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Effect of interface properties on the performance of CGS heterojunction solar cells

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In the tandem solar cells based on CGS (ZnO/CdS/$CuGaSe_2$) single solar cells, we have the interface state density of defects between CdS buffer layer and $CuGaSe_2$ absorber layer witch causes undesirable carriers recombination, Gaussian distribution model describe this interfacial recombination witch depending to interface state density. In this work we simulated the effect of the interface state density in the buffer and absorber layer of ZnO/CdS/$CuGaSe_2$ solar cells that is variated from 10^{14} to 10^{18} cm^{-3} on I-V characteristics and efficiency. We used the wxAMPS simulator to get the results.

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1. Introduction

Many research groups are worked on tandem chalcopyrite solar cells including the thin film CGS like the tandem solar cells CGS/CIGS with conversion efficiency (η) of 25.1 % [1]. Also a tandem solar cell CGS/CIS with conversion efficiency (η) equals 24.1 % [2]. The single solar cells CGS leads the totality of conversion efficiencies 18.22 %, 17.5 % in the tandem CGS/CIGS and CGS/CIS respectively [1-2], therefor it is important to study this CGS single solar cells.In the CGS chalcopyrite solar cells (ZnO/CdS/$CuGaSe_2$) we have the interface state density in the absorber ($CuGaSe_2$) and buffer (CdS) layer due to defects witch reduce the performances, the interface recombination at a heterojunction interface is the main loss mechanism in heterojunction solar cells.

We use the wxAMPS simulator [3] to see the influence of this interface state density at the absorber and buffer layer of CGS solar cells, we must kept all the parameters of ZnO/CdS/$CuGaSe_2$ structure constant and varying the interface state density at the buffer layer then the absorber layer, for each value of interface state density NIA (a-CdS), NID (d- $CuGaSe_2$) we draw the I-V plot and calculate the efficiency, finally we find the main responsible layer to interfacial properties.

2. Model description

To understand this interfacial properties we tried to give a simple device model of CGS solar cells. The ZnO window layer is used to minimize the defect density of the surface, Table.1 shows the schematic of thin film CGS solar cell design studied in this work.

Table 1. CGS solar cells schematic structure.

Front contact ZnO	Nd =1x10^{18} cm^{-3}	(0.1µm)
Buffer layer n-CdS	Na=2x10^{18} cm^{-3}	(0.05µm)
Absorber layer p-CGS	Nd =1x10^{14} cm^{-3}	(0.250µm)

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This CGS device structure is governing by the Poisson's equation (1), continuity equation (2) for the electrons and continuity equation (3) for the hole [4].

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

where n, p are the concentrations of free electrons and holes, N_D^+, N_A^- are the ionized concentrations donors and acceptors respectively, nt, pt are the concentrations of trapped electrons and holes, Ψ is the electrostatic potential, ε is the dielectric permittivity of semiconductor, and q is the electron charge.

$$\frac{1}{q}\frac{dj_n}{dx} = R(x) - G(x) \qquad (2)$$

$$\frac{1}{q}\frac{dj_p}{dx} = G(x) - R(x) \qquad (3)$$

where, jn, jp are electron and hole current density, the term R is the net recombination rate resulting from band-to-band and G is the optical generation rate, the functions (2) and (3) with their boundary conditions are detailed in AMPS 1D manual [5]. The interfacial recombination model for the defects implemented in wxAMPS simulator, this model is based on Gaussian distribution witch depending to interface state density NIA and NID, the standard energy deviation WGA and WGD, the peak energy position EGA and EGD and the capture cross sections σn, σp both of electrons and holes.

3. Effect of interface state density on performences of CGS solar cells

Under AM1.5G spectrum light the CGS single solar cells can achieve efficiency of 18.92 % with 0.260 µm of thickness absorber layer [6]. In this simulation we put 0.250 µm of thickness absorber layer, AM1.5G spectrum light and surface recombination velocities of both electrons S_e and holes S_h respectively equal to 10^7 cm/s. The absorption coefficient of ZnO and CdS are taken from Ref [7] and CGS is taken from Ref [8]. All the parameters used in this simulation are given in table 2.

Table 2. Material parameters used in this simulation [6-7].

Layer properties	**ZnO**	**CdS**	**CGS**
Permittivity	9	10	13.6
Electron mobility (cm^2/vs)	100	100	100
Hole mobility(cm^2/vs)	25	25	25
Effective state density of electrons Nc (cm^{-3})	$2.2x10^{18}$	$2.2\ x10^{18}$	$2.2\ x10^{18}$
Effective state density of holes Nv (cm^{-3})	$1.8\ x10^{19}$	$1.8\ x10^{19}$	$1.8\ x10^{19}$
Band gap Eg (ev)	3.3	2.4	1.69
Electron affinity χ (ev)	4.4	4.2	4.8
Interface state density NIA, NID (cm^{-3})	10^{17}	Variable	variable
Peak energy position EGA, EGD(ev)	1.65	1.2	0.84
Standard energy deviation WGA, WGD (ev)	0.1	0.1	0.1
Electron capture cross section σn (cm^2)	$1x10^{-12}$	$1x10^{-17}$	$2x10^{-15}$
Hole capture cross section σp (cm^2)	$1x10^{-15}$	$1x10^{-12}$	$3x10^{-13}$

First case we give the interface state density to absorber layer NID=10^{17} cm^{-3} and varying the interface state density of buffer layer NIA from 10^{14} to 10^{18} cm^{-3}. Second case we fix the interface state density of buffer layer to NIA=10^{17} cm^{-3} and varying the interface state density of absorber layer NID from 10^{14} to 10^{18} cm^{-3}, we compare the results.

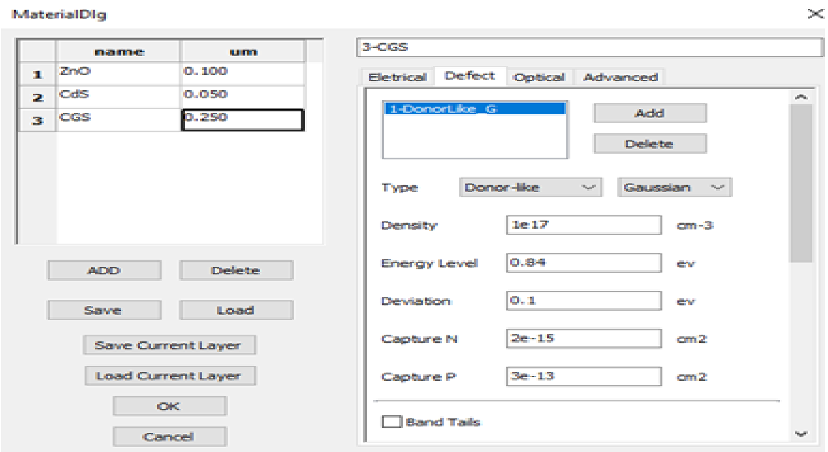

Fig 1. wxAMPS simulator interface.

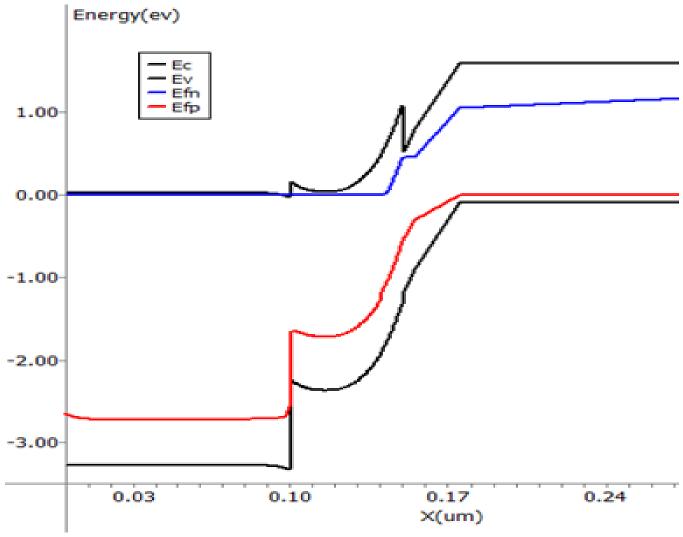

Fig. 3. Band diagram of CGS solar cells with interface state density both of baffer and absorber later NID=NIA=10^{17} cm^{-3}.

4. Results and discussions

4.1 Effect of interface state density NIA on buffer layer of CGS solar cells

In the simulation, we have varied the interface state density NIA from 10^{14} to 10^{18} cm^{-3} the results are given in table 3.

Table 3. Result of interface state density variation at the buffer of CGS solar cells.

Interface state density NIA (cm^{-3})	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	Efficiency η (%)
10^{14}	1.06	20.83	82.97	18.47
10^{15}	1.06	20.65	82.73	18.25
10^{16}	1.06	19.91	82.22	17.47
10^{17}	1.06	19.46	81.93	16.96
10^{18}	1.02	18.95	77.31	15.09

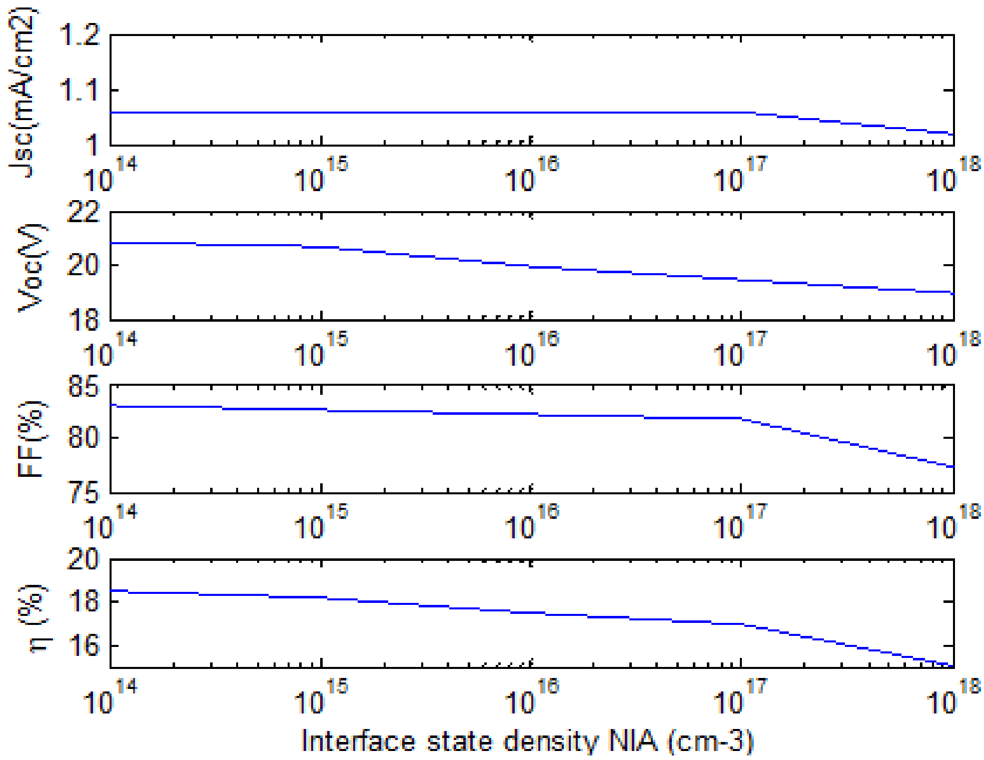

Fig. 4. Influence of interface state density NIA at the CGS buffer layer on photovoltaic parameters.

When we have the a interface state density at the buffer layer NIA= 10^{14} cm^{-3} , the fill factor gets the maximum value which equals to 82.97 %, J_{sc} = 20.83 mA/cm^2 and V_{oc}=1.06 V contrary when its takes 10^{18} cm^{-3} the fill factor decreases to 77.31%, J_{sc} = 18.95 mA/cm^2 and V_{oc} =1.02V. In general, the interface density state of buffer layer effects on the quality of I-V characteristics as showing in figure 5.

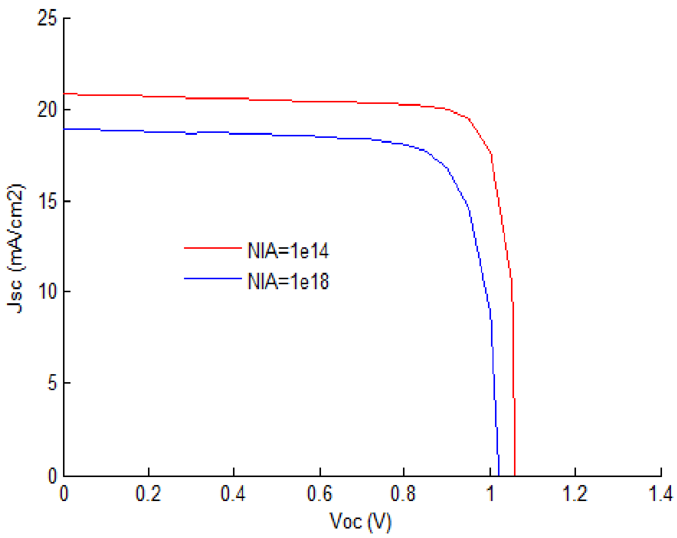

Fig. 5. Characteristics for high and low interface state density at the buffer layer of CGS solar cells.

4.2. Effect of interface state density NID on absorber layer of CGS solar cells

In this simulation, we have varied the interface state density NID from 10^{14} to 10^{18} cm^{-3} the results are given in table 3.

Table 3. Result of interface state density variation at the absorber of CGS solar cells.

Interface state density NID (cm^{-3})	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	Efficiency η (%)
10^{14}	1.22	19.67	85.70	20.66
10^{15}	1.20	19.67	84.66	20.12
10^{16}	1.14	19.65	82.51	18.61
10^{17}	1.06	19.46	81.93	16.96
10^{18}	0.83	18.85	59.78	9.41

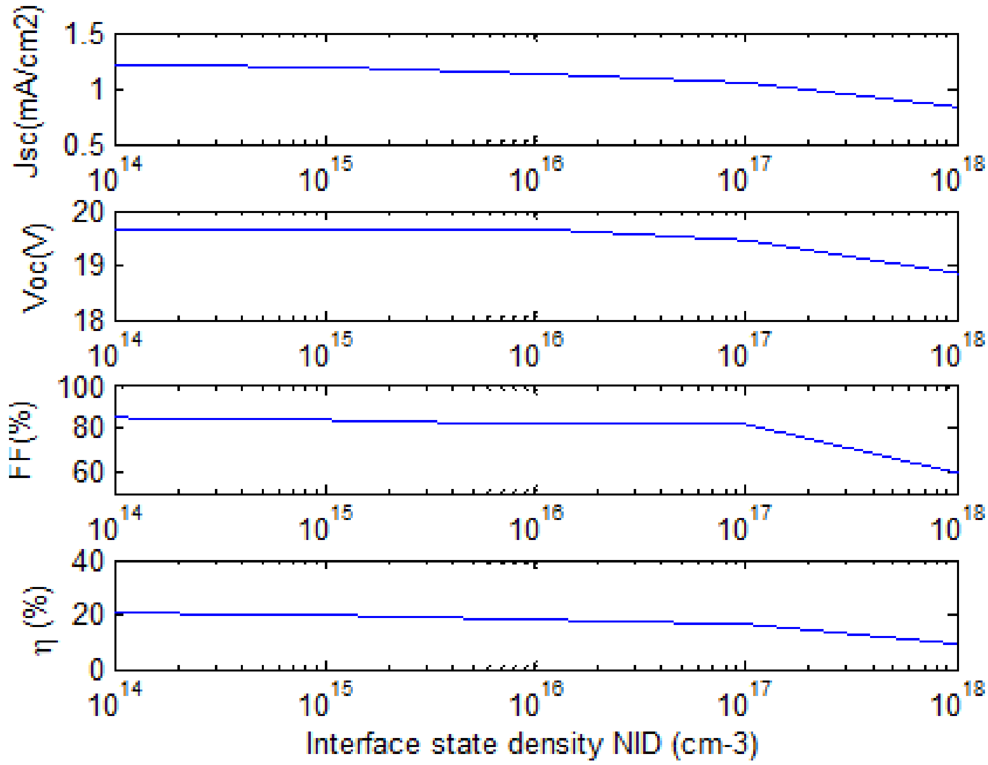

Fig. 6. Influence of interface state density NID at the CGS absorber layer on photovoltaic parameters.

It is clear that the increasing of interface state density of the absorber layer reduce the performance of CGS solar cells. When we have the a interface state density NID at the absorber layer equals to 10^{14} cm^{-3}, the fill factor gets the maximum value which equals to 85.70 %, J_{sc} = 19.67 mA/cm^2, V_{oc} =1.22 V when it takes 10^{18} cm^{-3} the fill factor decreases to 59.78 %. J_{sc} =18.85 mA/cm^2 V_{oc} =0.83 V. Also the interface density state at the absorber layer effects on the quality of I-V characteristics as showing in figure 7.

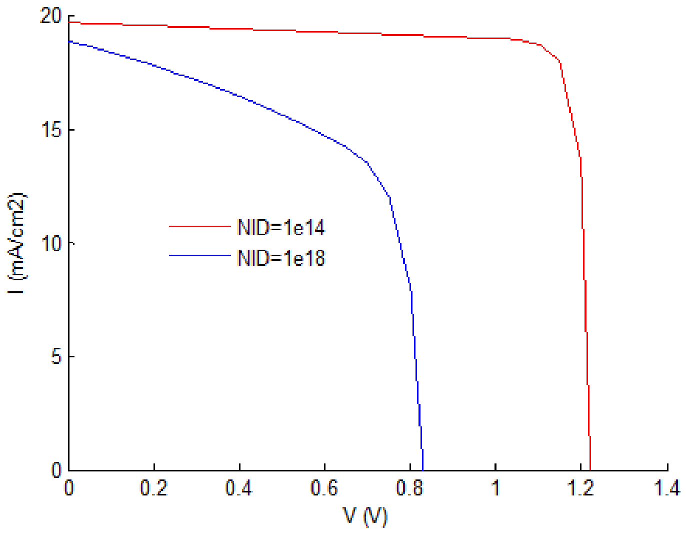

Fig 7. I-V characteristics for hight and low interface state density at the absorber layer of CGS solar cells.

The increasing of the interface density reduce the solar cell efficiency by providing new recombination energy levels in the semiconductor bandgap at the buffer and absorber which degrade the photovoltaic parameters of CGS solar cells, when the interface state density NID=NIA $=10^{17}$ cm^{-3} the J_{sc}= 19.46 mA/cm^2 and .V_{oc}= 1.06 V, if the interface at buffer layer NIA=10^{18} cm^{-3} the J_{sc}= 18.95 mA/cm^2 and V_{oc}= 1.02 V, we have a small changes. However, if the interface at absorber NID=10^{18} cm^{-3} the J_{sc}= 18.85 mA/cm^2 and V_{oc}= 0.83 V we have a big changes. For a hight interface state density the absorber layer have a big effects on efficiency of CGS solar cells figure 8.

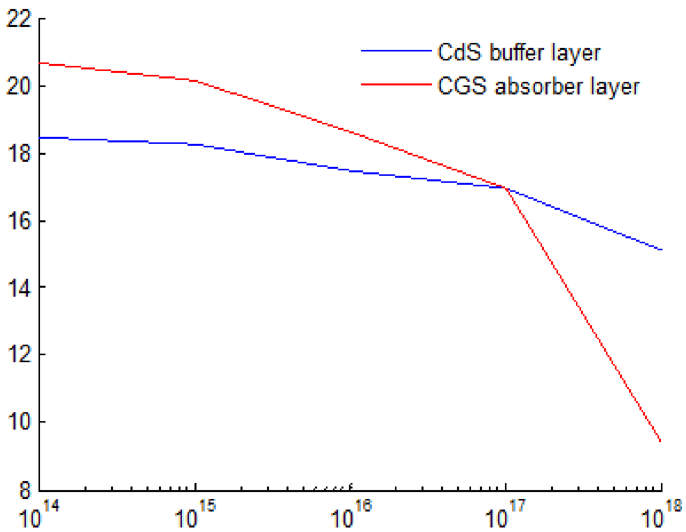

Fig. 8. Effect of interface state density both of buffer and absorber layer on the efficiency of CGS solar cells.

5. Conclusion

In this work, we demonstrated the effect of interface state density at the absorber and buffer layer on CGS solar cell parameters like open circuit voltage Voc, short circuit current density Jsc, fill factor FF and the conversion efficiency η. The conversion efficiency η will take the maximum value when we have a little interface state density of defects. For the interface state density of 10^{18} cm^{-3} at the buffer layer, the efficiency η is about 15.09 %, while for the interface state density of 10^{18} cm^{-3} at the absorber layer, the η is 9.41% . The efficiency η decrease in the highest interface state density values at the absorber layer. These observations lead us to conclude that to improve of the CGS performances solar cells we have to reduce the maximum of defects at the absorber of these chalcopyrite solar cells.

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