Influence of the doping of the absorber and the charged defects on the electrical performance of CIGS solar cells

SOCE Mouhamadou Mamour*, DIENG Moustapha **, EHEMBA Alain Kassine, DIALLO Demba**, WADE Ibrahima****

* Laboratory of semiconductor and Solar Energy; Physics Department, Faculty of Science and Technology University CHEIKH Anta DIOP, DAKAR-SENEGAL

** Laboratory of semiconductor and Solar Energy; Physics Department, Faculty of Science and Technology University CHEIKH Anta DIOP, DAKAR-SENEGAL

Abstract- In this paper, we have tried to show the importance of doping and defects charged on CIGS solar cells. Indeed according to our simulations, we could see that the electrical performance of these types of cells highly dependent on these two parameters. We also studied the dependence between doping and charged defects on the evolution of the electrical parameters. It was found that the results with neutral defects different from those charged with defects. The doping level for best performance (solar cell with Cu-poor absorber) is lowest with neutral defects than with the charged defects.

Index Terms- charged defect, CIGS, Cu-rich, Cu-poor, Doping.

I. Introduction

Solar cells based on $Cu(In,Ga)Se_2$ are currently the best thin film solar cells and are the only devices capable to rich photovoltaic conversion efficiencies near 22% [1]. This tells us about the future of these cell types, and improvement which it is subject. In these cell types, the absorber is the central element, and has several features whose final performance cell depends. First, defects that are either superficial or deep. Superficial defects may be linked to the doping of these materials and deep defects are often charged statements that are donors, acceptors or neutral.
Doping is very important in semiconductor materials. It strongly influences the efficiency. In the case of our study, doping CIGS is due to intrinsic defects: meaning the shortcomings and deficiencies of copper or selenium. The first type of gap will lead to a p-type material, and the second to n-type material. [2]
So far CIGS solar cells with doped p-type absorber give a higher yield. In reality, this corresponds to the Cu-poor material. In various studies, they found that doping varies depending on the copper content in the material. Thus the Cu-rich absorber will be much doped but will have a lower efficiency caused by the recombination at the interface absorber / buffer layer [3].
In the following we will try to model and simulate the observations using SCAPS.
First we will do the simulation of a solar cell with different doping concentration of the absorber but considering the deep flaws as neutral (which do not exist in reality) and then consider the case or deep defects will charged.

II. Modeling using SCAPS

Our model is based on CIGS Numos Baseline SCAPS but with some modifications. We will vary the doping 10^{14} to 10^{18} cm^{-3} and see the evolution of the electrical parameters. We will consider two cases: the first WERE defects are considered neutral, and the second defects will be charged. All simulations are performed at a temperature of 300 K. Illuminated characteristics have been simulated under AM1.5G illumination conditions with a power density of 100 mW/cm^2.

1. PRESENTATION SCAPS

SCAPS has been designed to simulate CIGS and CdTe based solar cells. It is developed at the Department of Electronics and Information Systems (ELIS) of the University of Gent and is freely available to the photovoltaic community since 1998 [23]. The main functionality of all semiconductor software packages in general, and SCAPS in particular, is to solve the system of partial differential equations formed by the Poisson (1) equation and the continuity equations for electrons (2) and holes (3) [4].

$$\frac{\partial}{\partial x}\left(\varepsilon_0 \varepsilon \frac{\delta \Phi}{\delta x}\right) = -q\left(p - n + N_D^+ - N_A^- + \frac{\rho_{def}}{q}\right) \quad (1)$$

$$-\frac{\partial Jn}{\partial x} - U_n + G = \frac{\partial n}{\partial t} \quad (2)$$

$$-\frac{\partial Jp}{\partial x} - U_p + G = \frac{\partial p}{\partial t} \quad (3)$$

The derivatives with respect to time disappear in the steady state regime and are replaced by a multiplication by *in* the small $j\omega$ signal analysis.
The terms of current density Jn et Jp are respectively given by equations (4) and (5) when the tunnel effect is not consider; if not other terms can be added.

$$Jn = -\frac{\mu_n n}{q}\frac{\partial E_{Fn}}{\partial x} \quad (4)$$

$$Jp = +\frac{\mu_p p}{q}\frac{\partial E_{Fp}}{\partial x} \quad (5)$$

2. WITH NEUTRAL DEEP DEFECTS.

Table 1 shows our simulation parameters. Table 2 gives the properties of the interface p-Cu (In, Ga) Se $_2$ / n-CdS and different layers.

Tableau 1: Cu (In, Ga) Se $_2$ Solar Cell Parameters

Parameters	p-Cu (In, Ga) Se_2 Absorber	n-CdS Buffer	i-ZnO Window	n-ZnO Window
d [nm]	3000	50	50	200
ε_r	13.6	10	9	9
χ [eV]	4.5	4.2	4.45	4.45
E_g [eV]	1.1	2.4	3.3	3.4
ν_n [cm/s]	10^7	10^7	10^7	10^7
ν_p [cm/s]	10^7	10^7	10^7	10^7
μ_N [cm^2/Vs]	100	100	100	100
μ_P [cm^2 /Vs]	25	25	25	25
$\|N_A-N_D\|$ [cm^{-3}]	10^{14} ; 10^{15};10^{16}; 10^{17} or 10^{18}	10^{17}	10^{18}	10^{18}

Tableau 2: Bulk Defect and Interface Properties

	p-Cu (In,Ga)Se_2 Absorber	Interface	n-CdS Buffer	i/n-ZnO Window
Energy level ΔE [eV]	0.6	uniform	midgap	midgap
Charge type	neutral	neutral	neutral	neutral
Total defect density N (/cm^3 or cm^2)	1.77210^{13}	10^{10}	1.77210^{17}	1.77210^{16}
Capture Cross-Section electrons [cm^2]	510^{-13}	10^{-19}	10^{-13}	10^{-12}
Capture Cross-Section holes [cm^2]	10^{-15}	10^{-19}	10^{-13}	10^{-12}

3. WITH CHARGED DEEP DEFECTS.

To show the influence of the charge of deep defects, we will make the simulation by changing the types of charge and always varying the doping level of the absorber of 10^{14}-10^{18} cm^{-3}. Table 1 will be unchanged against for Table 2 type's charges will be amended and give the table 3.

Table 3: Bulk Defect and Interface Properties

	p-Cu (In,Ga)Se_2 Absorber	Interface	n-CdS Buffer	i/n-ZnO Window
Energy level ΔE [eV]	0.6	uniform	midgap	midgap
Charge type	Donor	neutral	Acceptor	Acceptor
Total defect density N (/cm^3 or cm^2)	1.77210^{13}	10^{10}	1.77210^{17}	1.77210^{16}
Capture Cross-Section electrons [cm^2]	510^{-13}	10^{-19}	10^{-13}	10^{-12}
Capture Cross-Section holes [cm^2]	10^{-15}	10^{-19}	10^{-13}	10^{-12}

III. RESULTS AND INTERPRETATION

1. WITH NEUTRAL DEEP DEFECTS

From Tables 1 and 2, we get the results on some electrical parameters namely: the open circuit voltage Voc (V), the short circuit current Jsc (mA / cm^2), the fill factor FF (%) the efficiency η (%). These results are shown in Table 4.

Table 4: Results of simulations in to doping absorber with defects neutrals.

Doping (cm^{-3})	Voc (Volt)	Jsc (mA/cm^2)	FF (%)	η(%)
10^{14}	0.518030	36.79572131	78.3783	14.9399
10^{15}	0.547860	35.47898371	77.6218	15.0877
10^{16}	0.596261	33.70005166	79.4583	15.9664
10^{17}	0.652234	32.34225465	70.9898	14.9751
10^{18}	0.7522999	10.61594310	18.6805	1.4919

Figures 1 (a), 1 (b) and 2 (c), 2 (d) respectively show the changes in the open circuit voltage, short circuit current, the fill factor and the efficiency according to doping. In Figure 1 (a) there is an increasing trend of Voc depending on the doping of the absorber. The Cu-rich absorbers are more doped than the Cu- poor absorbers.

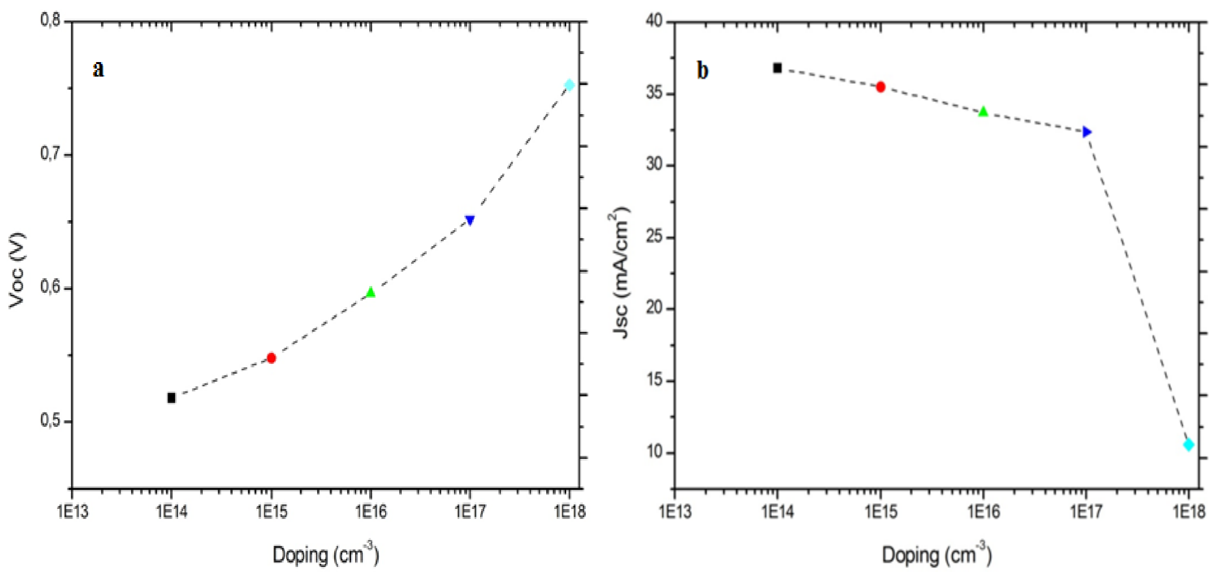

Figure 1: Variation of Voc (a) and the Jsc (b) according to doping.

Indeed a strong doping implies a value of Voc most important, this tells us about the interest of doping of the absorber on the electrical performance of CIGS solar cells. The transport properties of recombination are better in the Cu-rich absorber, which should give a cell with rich absorber Cu much more efficient [3].

However if you look closely the evolution of the performance of the cell (c), although the latter is maximum rating when the absorber is less doped (10^{16} cm^{-3}). And so the solar cell with Cu-poor absorber gives a greater efficiency. This situation can be explained by the fact that a high doping density may cause the reduction of carrier life time and at the same time the current as we shown in Figure (b) [5]. There is a decrease in the short circuit current depending on the degree of doping of the absorber, of Cu-poor cell in the Cu-rich cell.

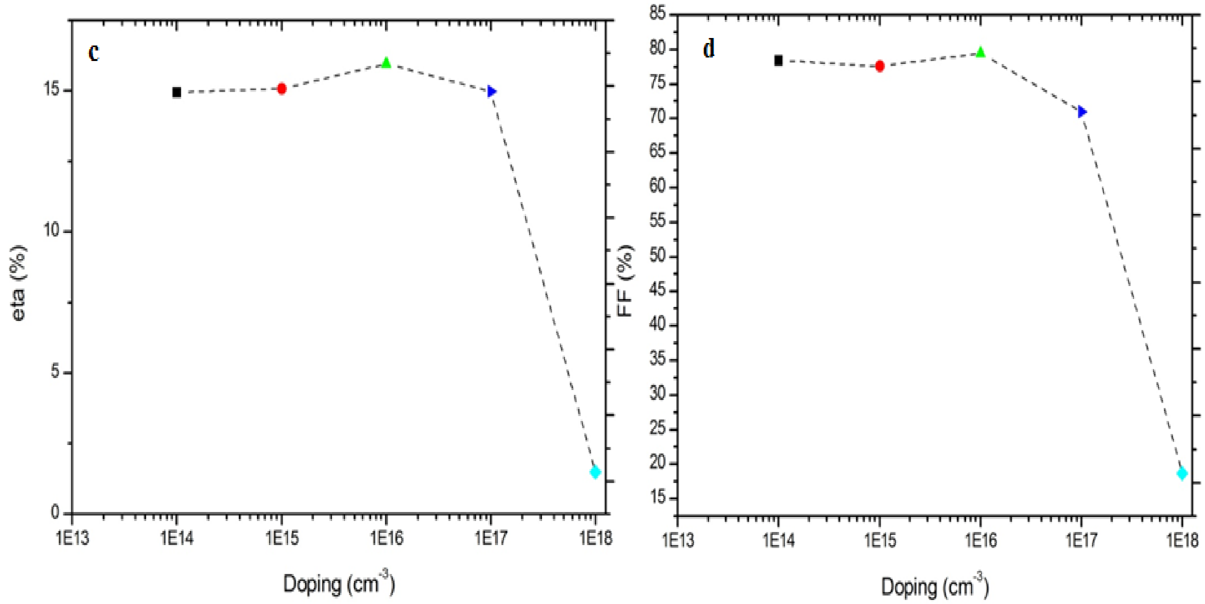

Figure 2: Variation of efficiency η (%) **(c)** and the fill factor FF(%) **(d)** according to doping.

2. WITH CHARGED DEEP DEFECTS

In this part, we have done the simulations considering the deep defects as charged. Table 3 was used. The results are shown in Table 6.

Table 6: Results of simulations in to doping absorber with charged defects.

Doping (cm^{-3})	Voc (Volt)	Jsc (mA/ cm^2)	FF (%)	η (%)
10^{14}	0.522790	37.00283318	63.1109	12.2086
10^{15}	0.554241	35.59585529	61.8635	12.2048
10^{16}	0.610461	33.72192436	53.6887	11.0523
10^{17}	0.705010	31.38062396	22.3044	4.9345
10^{18}	0.790470	5.22898026	31.3583	1.2962

With the change of the types of defects, there is a general decrease in electrical parameters, but moving in the same direction as if the defects were neutral except for the fill factor. For this, a significant decrease is observed at $10^{16}cm^{-3}$. The fact that a decrease of the electrical parameters is because with neutral defects were not recombination of minority carriers into the bulk of the absorber against the defects responsible for the recombination is important. Same is observed fluctuations and donor-acceptor transitions.

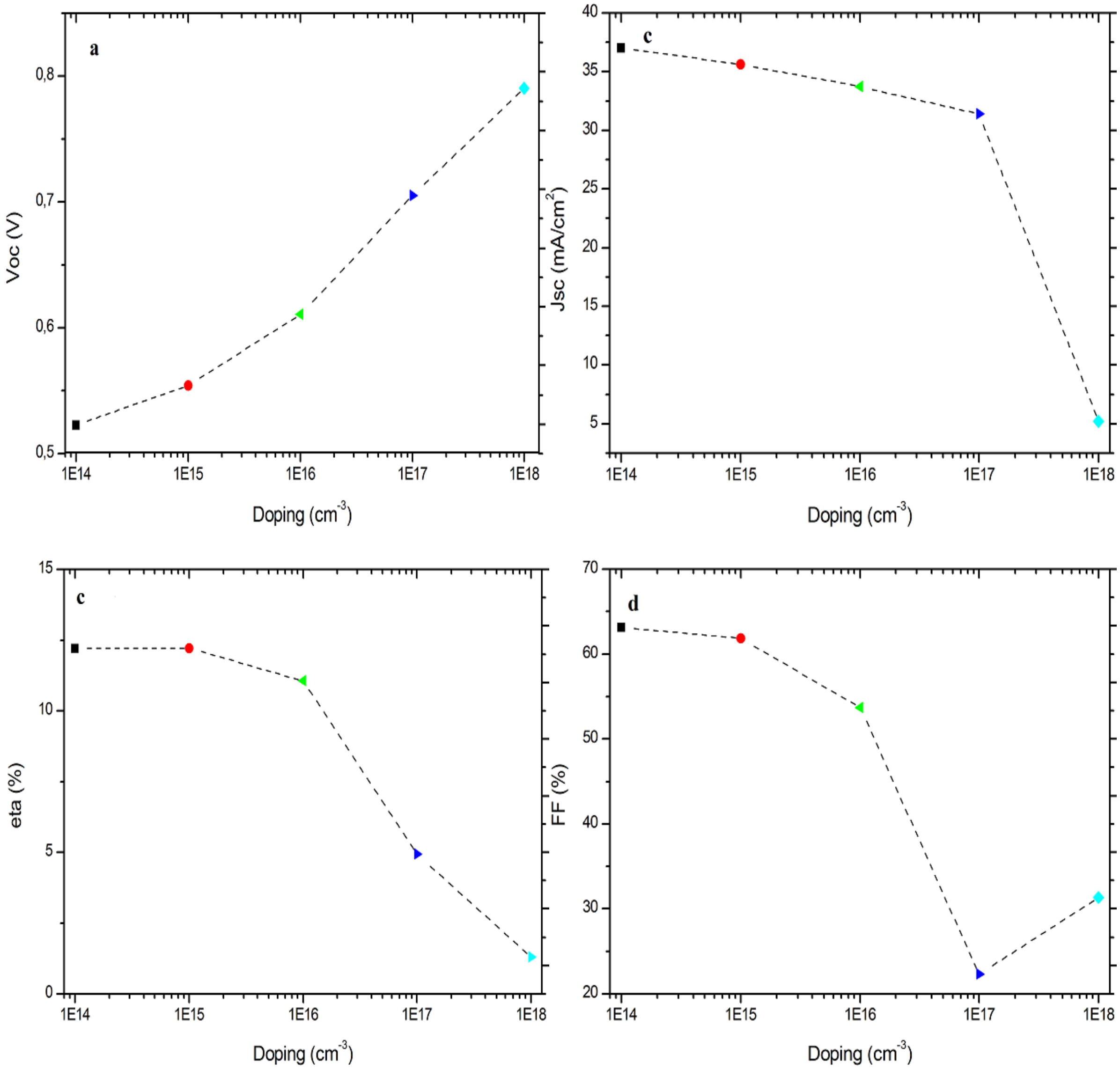

Figure 3: Variation in electrical parameters according to doping: Voc (a); Jsc (b); η (c); FF (d).

Here, the best efficiency is obtained for doping between 10^{14} and 10^{15}cm-3. Currently the best efficiency is always obtained with the cell with a Cu-poor absorber, although Cu-rich absorbers have more good transport properties. The change of the charge defect has the major effect of reducing the doping level of the best cell efficiency.

IV. CONCLUSION

This study allowed us to understand the interests of doping and charge defects on CIGS solar cells. Thus it has been found that the electrical parameters always increases when a cell is going on with an absorber whose underlying defects in a cell are charged with absorber whose defects are neutral in part due to the decrease in the recombination of minority carriers at the bulk of the absorber. It has also been seen that the change of the charge defect has the major effect of reducing the doping level of the best cell efficiency.
To obtain CIGS solar cells of high performance, it will minimize the maximum defects at the mass of the absorber and recombination phenomena at the interface absorber /buffer layer.

ACKNOWLEDGMENT

To all members of the team thin layers of Solar Energy, Materials and Systems Laboratory (LASES), Marc BURGELMAN University of GENT in Belgium for the software SCAPS.

REFERENCES

[1] P. Jackson, D. Hariskos, R. Wuerz, O. Kiowski, A. Bauer, T.M. Friedlmeier and M. Powalla, Phys. Status Solidi RRL, (2015).

[2] A-Ras, D., G. Kostorz, D. Bremaud, M. Kalin, F.V. Kurdesau, A.N. Tiwari, and M. Dobeli, *Formation and characterisation of MoSe2 for Cu(In,Ga)Se2 based solar cells.*Thin Solid Films, 2005. **480**: p. 433-438.

[3] S. Siebentritt*, L. Gütay, D. Regesch, Y.Aida, V. Depredurand, *Why do we make Cu (In, Ga) Se2 solar cells non-stoichiometric?* 2013, pp.18-19-20-21.

[4] K. Decock, Defect Related Phenomena in Chalcopyrite Based Solar Cells, 2012, Université de GENT, Belgique.

[5] R. Scheer and H-W. Schock, *Chalcogenide Photovoltaics*, Physics, Technologies, and Thin Film Devices, 2011 wiley-vch, Verlag & Co. KGaA, Boschstr. 12, 69469 Weinheim, Germany.

AUTHORS

First Author –SOCE Mouhamadou Mamour, PHD student, University CHEIKH Anta Diop-Dakar, LASES,kifamamour@gmail.com
Second Author – DIENG Moustapha, Professor and Thesis Director, University CHEIKH Anta Diop-Dakar, Physics Department, LASES, diengmoustapha@hotmail.fr
Third Author – EHEMBA Alain Kassine, Doctor, University CHEIKH Anta Diop of Dakar Physics Department, LASES
Fourth Author–DIALLO Demba, PHD student, University CHEIKH Anta Diop of Dakar Physics Department, LASES
Fifth Author –WADE Ibrahima, PHD student, University CHEIKH Anta Diop of Dakar, Physics Department, LASES

Correspondence Author – SOCE Mouhamadou Mamour, Email: kifamamour@gmail.com, Contact number: 00221772011281.