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# Impact of [Ga]/[In+Ga] Ratio on the Generation-Recombination Rates of $Cu(In,Ga)Se_2$ Solar Cells

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*Abstract*— **The changes in the performance that happen in the cells when varying the Ga content are discussed using simulation program Solar Cell Capacitance Simulation one-dimensional (SCAPS-1D). The efficiency of the solar cells reaches a maximum value when Ga concentration at the junction reaches x=0.3 due to the minimum defect concentration in the absorber at x=0.3; beyond this value, the increase of the ratio x becomes detrimental and the efficiency drops drastically. The effect of the [Ga]/[(In+Ga)] ratio (x) for different absorber thickness on the generation and recombination rates is analyzed. The results exhibit that the carrier generation rates decrease with increasing x in the CIGS bulk due to the enhancement of the band gap and therefore the defect concentration in the absorber. As the cells thickness is reduced the effect of the x becomes more important. For the thick layers the dominant recombination mechanism is in the bulk. However, for thinner ones the dominant recombination is in the space charge region (SCR). The recombination rates are hardly affected by the x when increasing the thickness of the absorber due to the lower absorption at the back contact for thick layers.**

*Keywords*— **CIGS; Generation; Recombination; [Ga]/[Ga+In] ; SCAPS**

## I. INTRODUCTION

Currently Cupper Indium Diselenide $CuInSe_2$ (CIS) solar cells have attracted interest for spatial applications because of the stability of CIS against electron and proton irradiation then the silicon or III-V semiconductors. The importance of the absorber layer band gap is not deniable for improving the performance of the solar cells, due to its impact on the absorption coefficient and therefore on a both generation and recombination of electrons and holes at the bulk of the absorber which leads to change the parameters of cell. $CuInSe_2$ (CIS) is an I-III-VI compound with a chalcopyrite structure. It is a direct band gap semiconductor material and has a large absorption coefficient ($10^5$ $cm^{-1}$) [1]. The ideal band gap for the solar spectrum is 1.4 eV [2]. $CuInSe_2$ has a lower-than-optimal band gap of 1.02 eV [3], and, because of that, the best CIS cells have achieved efficiencies of 15%. To raise the band gap to values more suitably matched to the AM1.5 solar spectrum, the $CuInSe_2$ compounds are alloyed with Gallium (Ga) to enhance its band gap which can be tuned from 1.04 eV (pure CIS) to 1.67 eV (pure CGS)) depending on the Ga content. Varying the [Ga]/[In+Ga] ratio in $CuIn_xGa_{1-x}Se_2$ material affects various parameters in the absorber such as band gap, optical absorption, and defect concentration which influence the performance of the solar cells.

In this study, numerical simulations of CIGS solar cells are carried out to investigate the effect the Ga content in CIGS absorber on the performance of solar cells as well as the effect of Ga content on the generation-recombination rates when the thickness of the active layer is reduced.

## II. MATERIALS PARAMETERS AND SIMULATION DETAILS

The CIGS solar cells structure used in this simulation is sketched in Fig.1. It is consists of the following layers: substrate soda lime glass (SLG); a Molybdenum (Mo), to realize an ohmic back contact; a p-CIGS absorber layer; an n-type buffer layer; typically CdS [4]; an undoped ZnO layer namely a transparent conduction oxide (TCO), and an Al:ZnO transparent front contact that has the same parameters of i:ZnO except the doping concentration which equal to $10^{20}$ ($cm^{-3}$). Metallic Ni/Al contact grids complete the cell. Input parameters of each layer in the cell are given in table 1. The absorber layer parameters employed in this simulation are kept unchanged except that the band gap energies, electron affinities, optical absorption ,and the bulk defect concentration which follows the model of Hanna et al [5] shown in Fig.2. these parameters are adjusted to the corresponding Ga mole fraction in the CIGS films [6].

In this work, the CIGS solar cells are modeled using the latest version (3.0.0.2) of the simulation program called: Solar Cell Capacitance Simulation one-dimensional (SCAPS-1D) [7-9]. This software tool that designed as a general polycrystalline thin-film device simulator and is mainly used

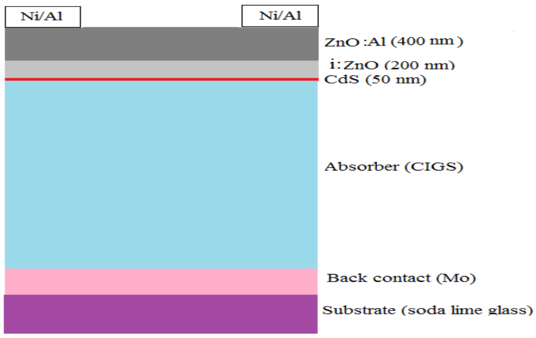


Fig.1 Schematic structure of CIGS based thin-film solar cells.

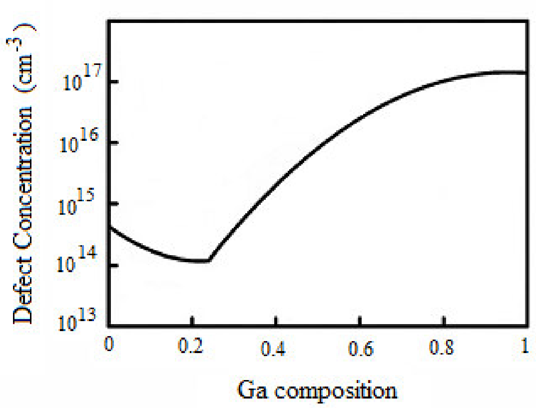


Fig.2 Variation of the defect concentration with Ga composition, x [5].

for modeling CdTe and CIGS/CIS based solar cells, allows the definition of thin-film solar cell devices stacks of layers with a large set of parameters and solves for each point the Poisson equation and continuity equations for electrons and holes:

$$\frac{d}{dx}J_n(x) - e\frac{\partial n(x)}{\partial t} - e\frac{\partial pn}{\partial} = G(x) - R(x) \quad (1)$$

$$\frac{d}{dx}J_p(x) + e\frac{\partial p(x)}{\partial t} + e\frac{\partial pn}{\partial} = G(x) - R(x) \quad (2)$$

Where $J_n$ and $J_p$ are electron and hole current densities, G(x) and R(x) are the generation and the recombination rates, respectively. Recombination in deep bulk levels and their occupation is described by the Shockley-Read-Hall (SRH) formalism. Recombination at the interface states is described by an extension of the SRH formalism, allowing the exchange of electrons between the interface state and the two adjacent conduction bands, and of holes between the state and the two adjacent valence bands [10-12]. All the bulk defects are at mid gap of the layers. The CIGS cell is simulated under AM1.5 spectrum irradiance with a power density of 100mW/cm$^2$ and at temperature of 300 K.

## III. Results and Discussion

### A. *Modelling with various [Ga]/[In+Ga] ratio*

As mentioned earlier, the CIGS has adjustable band gap

Table 1. CIGS solar cell input parameter values used for this simulation.

| Layer properties | | | |
|---|---|---|---|
| | **CIGS** | **CdS** | **i: ZnO** |
| W (μm) | variable | 0.05 | 0.2 |
| Eg (eV) | variable | 2.4 | 3.3 |
| χ (eV) | x=0: 4.57; x=1:3.98 | 4.45 | 4.55 |
| $\varepsilon/\varepsilon_0$ | 13.6 | 10 | 9 |
| $N_c$ (cm$^{-3}$) | 2*10$^{18}$ | 1.3*10$^{18}$ | 3.1*10$^{18}$ |
| $N_v$ (cm$^{-3}$) | 1.5*10$^{19}$ | 9.1*10$^{18}$ | 1.8*10$^{19}$ |
| $\nu_n$ (cm/s) | 3.9*10$^{7}$ | 3.1*10$^{7}$ | 2.4*10$^{7}$ |
| $\nu_p$ (cm/s) | 1.4*10$^{7}$ | 1.6*10$^{7}$ | 1.3*10$^{7}$ |
| $\mu_n$ (cm$^2$/Vs) | 100 | 72 | 100 |
| $\mu_p$ (cm$^2$/Vs) | 12.5 | 20 | 31 |
| doping (cm$^{-3}$) | 1*10$^{16}$ (a) | 5*10$^{17}$ (d) | 1*10$^{17}$ (d) |

by tuning the [Ga]/[Ga+In] ratio [13]. The variation of this ratio affects primarily the absorption coefficient within this material and consequently the generation-recombination rates. In this section, the ratio [Ga]/[ In + Ga] in $CuIn_{1-x}Ga_xSe_2$ is varied between 0 to 1 to show how this parameter affects the both cell performance and the generation-recombination rates. In this part, the thickness of the absorber is fixed at 2 μm. Figure 3 shows the performance of cell as a function of [Ga]/[ In + Ga] in termes of $V_{oc}$, $J_{sc}$, FF, and efficiency. The appearance of the trends in the parameters are very similar to that of the experimental results obtained by [14]. The short circuit current density ($J_{sc}$) decreased relatively linearly with increasing the Ga content, due to the decrease of absorption coefficient with increasing the band gap [15]. The open circuit voltage ($V_{oc}$) increased with the Ga content and reaches a saturation value at high Ga. The Fill Factor (FF) has lower values for the CIS (x=0) and CGS (x=1), and its optimal value is obtained around x = 0.5. the efficiency of the solar cell reaches a maximum value when Ga concentration at the junction reaches x=0.3; beyond this value, the increase of the ratio x becomes detrimental and the efficiency drops drastically. The simulation results are in good agreement with the results reported in the literature [15,16].

To elucidate the effects of the Ga ratio on the performance of the CIGS solar cells, the generation (G(x)) and recombination (R(x)) rates were studied as a function of the Ga content, x. Figure 4 (a) and (b) illustrate the depth-distribution curves of carrier generation rates and total recombination rates, respectively, for different Ga ratio. As can be seen, the carrier generation rates presented in the Fig.4 (a) decrease with increasing the depth in the absorber. However, increasing the Ga content reduces the initial value of the generation rates at the junction, due to the increase in the band gap which leads to lower absorption coefficients and a lack of absorption in the long-wavelength portion of the spectrum. This results explain obviously the decrease of the $J_{sc}$ in the Fig.3. Whereas the recombination rates decrease with increasing x, as shown in Fig.4 (b), until x reaches a value around 0.3, due to the decrease of the defect concentration as a function of Ga content. but, beyond this value, further the x is increased the recombination rates increased, due to the increase of the defect concentration as illustrated in Fig.2. Other the hand, increasing the Ga ratio affects much more the Space Charge Region (SCR) and the region beyond the SCR which means that the SCR recombination, in this case, is the dominant process. However, the back region is hardly affected by the variation of the Ga ratio. As the $V_{oc}$ depends essentially on the Ga content ( the band gap) of the SCR, increasing x leads to enhance the $V_{oc}$ which explains the results obtained in Fig.3. But, the high defects limit the enhancement of $V_{oc}$ which reaches a saturation value at high concentrations. The recombination rates in the others layers are independent of the absorber Ga content.

*B. Effect of [Ga]/[In+Ga] ratio with varying the absorber thickness*

CIGS has high absorption coefficient ($10^5 cm^{-1}$) [1] which permits to 0.5 µm of the absorber to absorb most than 90% of the incident photons. Today this material has a typical thickness of about 1.5-2 µm [17]. Various researches have reported the impact of the thickness of CIGS absorber layer on the cells parameters. The results show that as the thickness of the absorber is reduced the efficiency decreases. In the thin absorber layer compared to the thick ones the back contact and the depletion region become very close to each other which enhance the probability of the recombination carriers at the back contact. However, enhancing the band gap at the back surface mitigates this recombination. For this purpose the effect of the Ga content on the solar cell performance when varying the thickness of absorber from 0.5 µm to 2µm is studied. In Fig.5 we have reported the simulation results of the recombination rates versus the thickness of the absorber for

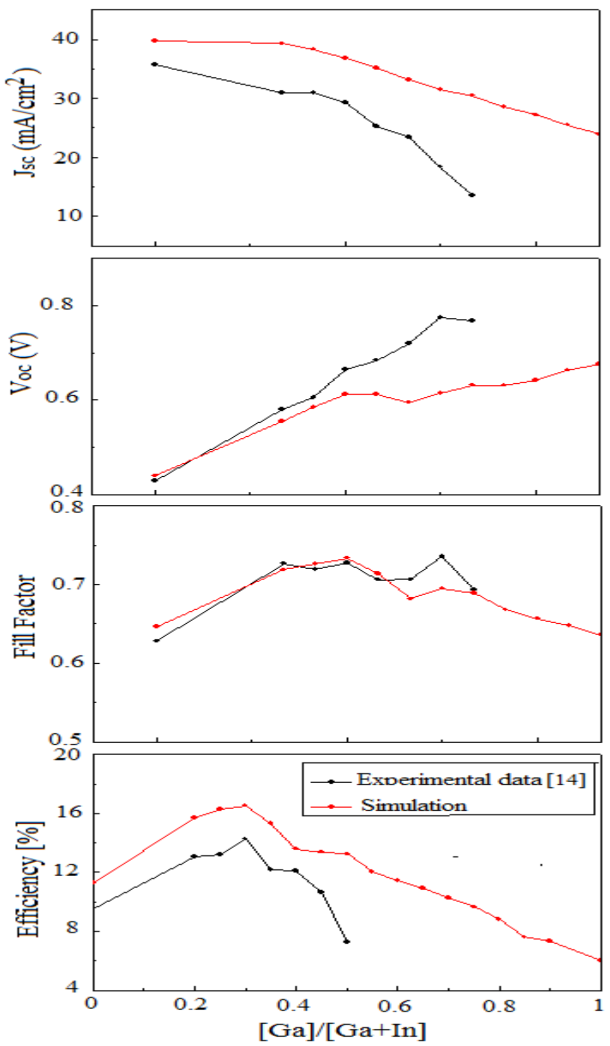


Fig. 3. Cell performance as a function of the Ga content.

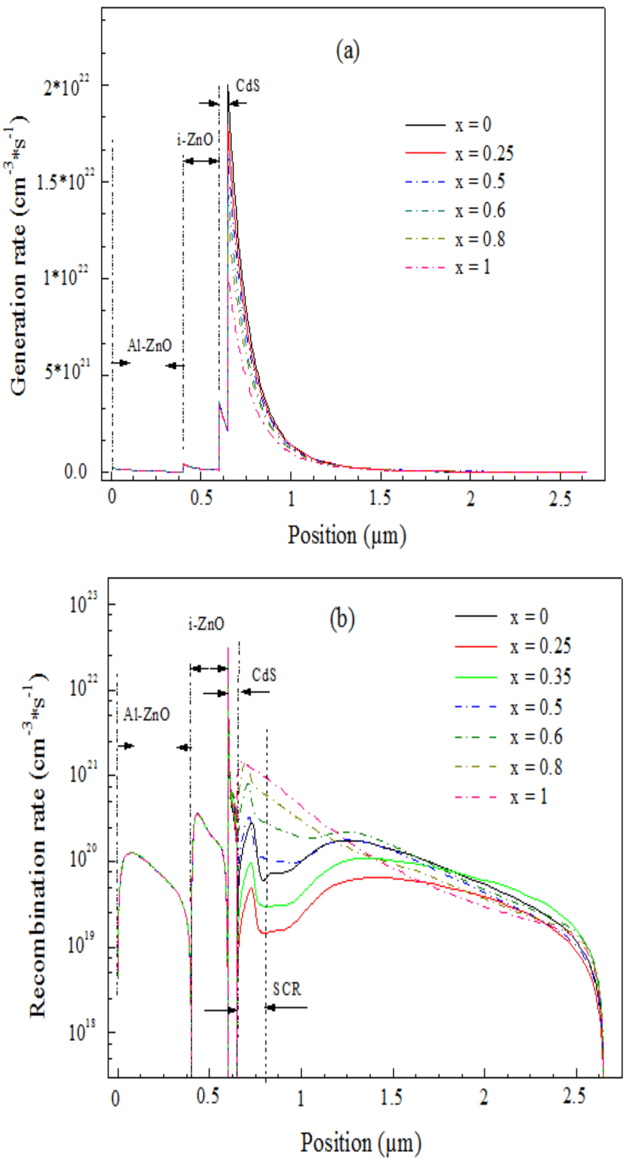


Fig. 4 The depth-distribution curves of (a) carrier generation rates and (b) total recombination rates of cells with various Ga/[Ga+In] ratio denoted (x).

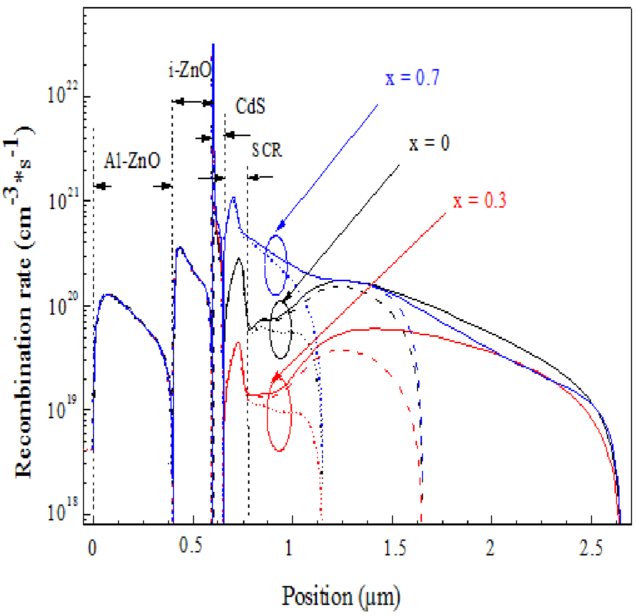


Fig.5. the depth- distributed curves of total recombination rates of cells with different [Ga]/[In+Ga] ratios at different thicknesses: solid lines, dashed lines and dot lines represent respectively 2µm, 1µm, and 0.5 µm.

different [Ga]/(In+Ga] ratio. The generation rates, not shown in this paper, decrease with decreasing the thickness and increasing the Ga content. For a lower x, when increasing the thickness, the dominant recombination mechanism is in the bulk of the absorber. However, for a thinner layer the recombination is in the SCR, because in these devices the depletion region becomes closer to the back surface when the thickness of the absorber is reduced, and therefore the [Ga]/[In+Ga] ratio at the back surface becomes important. As the thickness is reduced, the impact of the ratio x appears more when its value exceeds 0.3, where we remark that the recombination rates increase with increasing x, because the defect concentration overweights the increase of band gap at the back contact that expected to mitigates the recombination. The recombination rates are hardly affected by the x when increasing the thickness of the absorber. This can be attributed to the lower absorption at the back contact for thick layers, since 1.5 µm is enough to absorb all the solar spectrum incident photons [18].

## IV. Conclusions

In this work, the performances of CIGS solar cells have been simulated using the Capacitance Simulator in 1 Dimension SCAPS-1D. The relationship between the cell performance and the Ga ratio is revealed. The efficiency of the solar cell increases with the x lower than 0.3; beyond this value, the increase of Ga ratio becomes detrimental to the performance of the device. Also the effect of Ga content on the generation-recombination rates is presented. The results exhibit that carrier generation rates decrease with increasing x due to the decrease of absorption coefficient with increasing the band gap. However, the recombination ones have an optimum value around 0.3. Increasing x beyond this value enhance the recombination due to the increase of the defects concentration in CIGS solar cells by increasing Ga content. The effect of the Ga ratio for different absorber thickness on the generation and recombination rates is analysed. The recombination rates are hardly affected by the x when increasing the thickness of the absorber due to the lower absorption at the back contact for thick layers. As the cells thickness is reduced the effect of the x becomes more important, because the photoelectrons generated occur close to the back-contact. Moreover, for a lower x, for the thick layers the dominant recombination mechanism is in the bulk. However, for a thinner ones the recombination occurs in the SCR.

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