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Development and Simulation of a structure based on $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$ semiconductors alloys for a new generation of photovoltaic cells

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Abstract

The aim of our study is the development and simulation of thin films structure based on $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$ semiconductors alloys to improve the conversion efficiency of solar cells. We studied and simulated the variation effect of the Gallium concentration on some physical and electrical properties (lattice parameter, strain, energy gap, refractive index, absorption coefficient and $J(V)$ characteristic), this in order to optimize the best possible performances for solar cells. Then, we studied the influence of surface state density and temperature on solar devices characteristics. For better performance of our structure based on $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$, the concentration of gallium must be less than 40% and this to avoid the lattice mismatch with CdS buffer layer. We have demonstrated by simulation models the possibility for efficiency to reach 22% in the case of $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$ thin films solar cells.

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Keywords: Solar cells; Thin Films; $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$; Photovoltaics; Optoelectronics

1. Introduction

The copper indium diselenide, gallium (CIGS) is a multi-crystalline semiconductor of p-type with a high optical absorption coefficient. This material is used in heterojunction structures for thin film solar cells, often with a thin layer of n-type cadmium sulfide (CdS). The optimal band gap for a single junction solar cell is about 1.4eV. Pure CuInSe_2 has a gap equal to 1.04 eV [1]. To increase the width of the band gap,

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indium can be partially replaced by gallium and then we obtain the alloy of copper indium gallium diselenide (CIGS). When the percentage of gallium is in the margin of 20-40%, the Gap is equal to 1.1-1.2 eV, which gives the best efficiency for the solar cell. The band gap of pure CuGaSe₂ (CGS) is equal to 1.67 eV. The direct band gap and high absorption coefficient of CIGS gives the requirements for higher lifetime of minority carriers. This makes the CIGS material a suitable component for thin film solar cells. Solar cells based on CIGS were developed by several research teams and the record of efficiency was as high as 18.8% [2] at a laboratory scale. In terms of stability, the solar cells based on CIGS do not have the problem of degradation induced by light. Instead, they tend to have a slight increase in open circuit voltage and efficiency during the first hours of operation, but at the same time, they are more sensitive than, for example crystalline silicon solar cells to hot and humid environments [3]. Cu (In, Ga) Se₂ is considered one of the most promising materials used to manufacture low cost, high efficiency and large area of PV modules. The first commercial CIGS modules were reported in 1998 by 'Siemens Solar Industries', but their manufacturing is still on a limited scale. The success of this new generation of solar cells is linked to important research topics which are the decrease of indium concentration and the substitution of the thin layer of cadmium sulfide by a less dangerous material.

Nomenclature

a	lattice parameter of CuIn _{1-x} Ga _x Se ₂ in Angstrom unit Å
a ₀	lattice parameter of CdS in Angstrom unit Å
E _g	energy gap of the CuIn _{1-x} Ga _x Se ₂ in electron volt unit eV
b	Bowing parameter
E	incident photon energy in electron volt unit eV
α	absorption coefficient of the semiconductor in cm ⁻¹ unit
J	current density of the solar cell in mA/cm ² unit
J ₀	saturation current density of the solar cell device (diode) in mA/cm ² unit
q	electron charge in coulomb unit C
n	ideality factor of solar cell device (diode)
k	Boltzman constant in J/K unit
Φ(α)	photon flux in standard condition for PV modules test at AM 1.5 spectrum in W/m ² unit
η	energy conversion efficiency in % unit

2. Theory

In the case of CIGS solar cells we designed a heterojunction structure which consists of ZnO / CdS / CIGS. The layers of n-type layers are often called as "window", due to their transparency to the photon. Photons of energy <3.3 eV will pass through the ZnO window layer some 2.4 eV photon energy <E_{ph} <3.3 eV are absorbed in the CdS buffer layers, which was introduced in these cells for technology reasons, but most photons reach the CIGS layer and are strongly absorbed by CIGS semiconductor having direct gap with a very high absorption coefficient, so that the absorption length is very short. The

absorption is minimized by thinning damaging of this layer or alloying with other elements that increase the energy gap.

The density of CIGS varies with its composition because its crystal structure can change from the tetragonal form to the cubic one depending of Indium-Gallium ratio. If the mole fraction of gallium is below 0.5, then CIGS crystalline lattice get the structure of tetragonal chalcopyrite. Otherwise, if the mole fraction is above 0.5, the CIGS structure is cubic (zinc blende). Al-Bassam[4] has published two empirical formulas for the CIGS lattice parameters.

$$a_{\text{chalcopyrite}} = 5.75 - 0.33x \quad (1)$$

$$c_{\text{chalcopyrite}} = 11.45 - 0.40x \quad (2)$$

$$a_{\text{zincblende}} = 5.62 - 0.1x \quad (3)$$

The layer can be deformed for a certain thickness because of the disagreement of the lattice parameter between the CdS and CIGS layer. The theory of elasticity allows us to calculate the stress state of a film using the elastic constant. The various strains induced by the lattice mismatch are calculated from the following equation [5].

$$\varepsilon = \frac{a_0 - a}{a_0} \quad (4)$$

a is the lattice parameter of $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$ and a_0 that of CdS.

The band gap width of CIGS is mainly influenced by the concentration of gallium (Ga), but also by the concentration of copper (Cu). The Gap energy Measurements for CuInSe_2 revealed a value of about 1.01 eV at 300 K, but there are many differences between results. However, it is accepted that the Gap of CuIn_3Se_5 is 0.2 to 0.3 eV above the bandwidth of CuInSe_2 , a comprehensive review led to a value of 1.20 eV at 300 K. The band gap width of CuGaSe_2 (CGS) is about 1.65 eV. The band gap can be varied between the values of these two alloys which are CuInSe_2 and CuGaSe_2 . Energy Gap of the $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$ structure follows the relationship.

$$E_{g \text{ CIGS}} = (1-x)E_{g \text{ CIS}} + x.E_{g \text{ CGS}} - b.x.(1-x) \quad (5)$$

b is the Bowing parameter [6].

The absorption coefficient α of CuInGaSe_2 is very high, above $10^5/\text{cm}$ for higher energy photons more than 1.4 eV [7]. In many studies it was found that the fundamental absorption is well described by [8].

$$\alpha = \alpha_0 \frac{\sqrt{E - E_g}}{E} \quad (6)$$

Where E is the incident photon energy and α is the material constant for a type of semiconductor band gap direct. The proportionality constant α_0 depends on the density of states associated with the absorption of photons. The absorption coefficient depends on the material and also the wavelength of

light that is absorbed. The semiconductor materials have a sharp edge on their absorption coefficient, since the light has energy below the energy gap, not enough energy to lift an electron across the band gap. Therefore, this light is not absorbed.

The current density (J), defines the electric current through the cross section and its unit is A/m², but usually the used unit is mA/cm². The equation of the diode can be expressed using the current density:

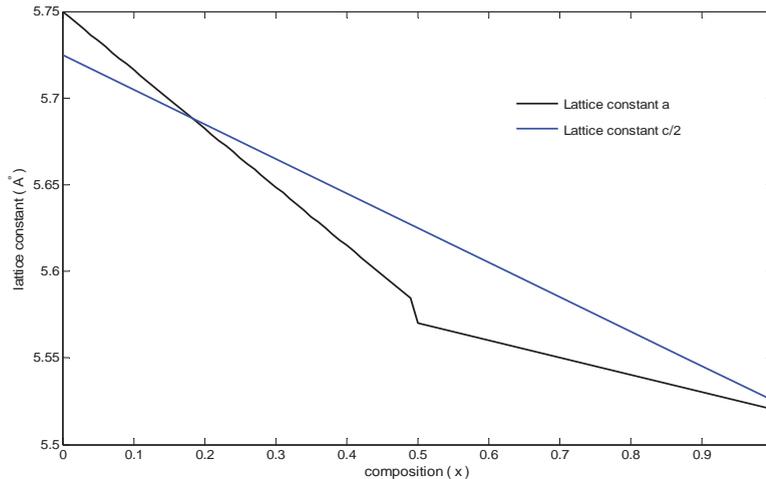


Fig. 1. variation of lattice parameter according to Gallium composition in CuIn_{1-x}Ga_xSe₂ structure

$$J = J_0 \exp\left(\frac{qV}{nKT} - 1\right) - J_{cc} \tag{7}$$

Where J₀ mA/cm² is the density of saturation current of the diode, V is the voltage applied to the cell, J the resulting current density, q the electron charge, n the ideality factor and k is the Boltzmann constant.

$$J_0 = J_{00} \exp\left(\frac{-E_g}{nKT}\right) \tag{8}$$

$$J_{cc} = \int_0^\infty E \cdot QE(\lambda) \phi(\lambda) d\lambda. \tag{9}$$

Where $\phi(\lambda)$ is the photon flux to the Air Mass Coefficient (AM) of spectrum in standard PV modules test conditions referenced AM 1.5 [9-13].

The open circuit voltage is the voltage at zero current. The open circuit voltage is equal to the difference in quasi-Fermi levels for electrons and holes between the two sides of V_{co} cell is given by:

$$V_{co} = \frac{E_g}{q} + \frac{nKT}{q} \ln\left(\frac{J_{00}}{J_{cc}}\right) \tag{10}$$

J₀₀ is a pre factor and 1 < n < 2

The efficiency of the solar cell is the ratio of maximum power and incident light power:

$$\eta = \frac{J_m V_m}{P_{light}} \tag{11}$$

The spectrum AM 1.5 corresponds to $P_{light} = 100 \text{ mW} / \text{cm}^2$.

3. Results and Discussion

The Fig 1 shows the evolution of the lattice parameter according to the composition of Gallium. We notice that the increase of Gallium composition decreases the lattice parameter. The influence of Gallium composition on the strain is illustrated by the Fig 2. We find that for $x = 0\%$, we have a lattice mismatch of 1%. For $x = 100\%$, we have a lattice mismatch of 5%. Thus, we can use this deformation to improve light absorption.

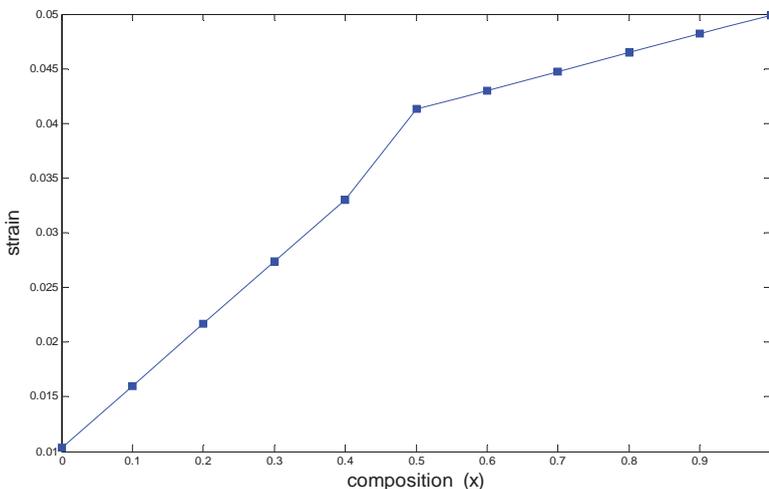


Fig. 2. variation of strain as a function of the composition of Gallium (x)

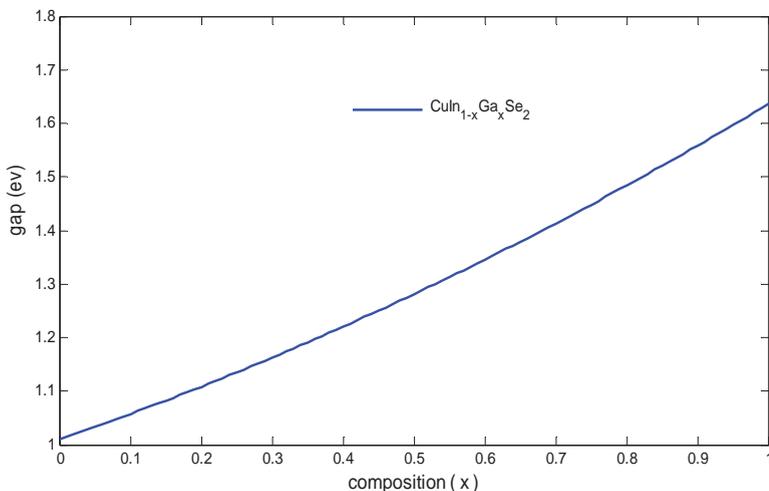


Fig. 3. band gap energy variation according to the concentration of Gallium

Fig 3 shows the variation of the band gap energy depending on the composition of Gallium; we see that the Gallium increase the energy of the gap. The gap of the structure $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$ increases by 40% by varying x from 0 to 100%, so there is a major Gallium influence on the solar cell characteristics. This effect increases the range of Gap, so we have a wide range of wavelengths that can be absorbed. The Fig 4 shows the evolution of the absorption as a function of incident photon energy. The absorption decreases with increasing the composition of Gallium. It has a significant absorption for compositions below 30%. Then, we plot the variation of characteristics J (V) which shows that the increase of open circuit voltage V_{oc} with increasing the composition of gallium against by the current density decrease as represented on Fig 5. The Fig 6 shows the evolution of the efficiency of the structure according to the composition of Gallium, for different temperatures and shows that the efficiency increases with increasing the composition of Gallium but decreases with temperature. For 40% Gallium composition at a temperature of 300K the cell efficiency reaches 21.45%.

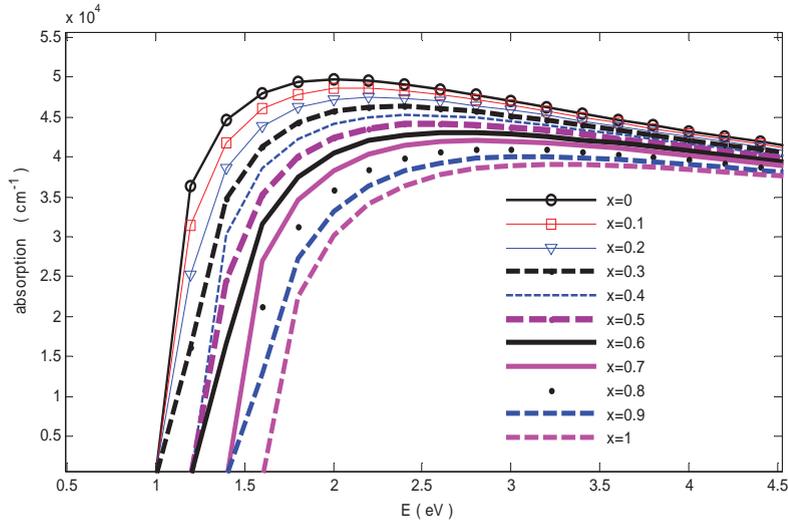


Fig. 4. absorption evolution as a function of incident energy for different Gallium composition (x)

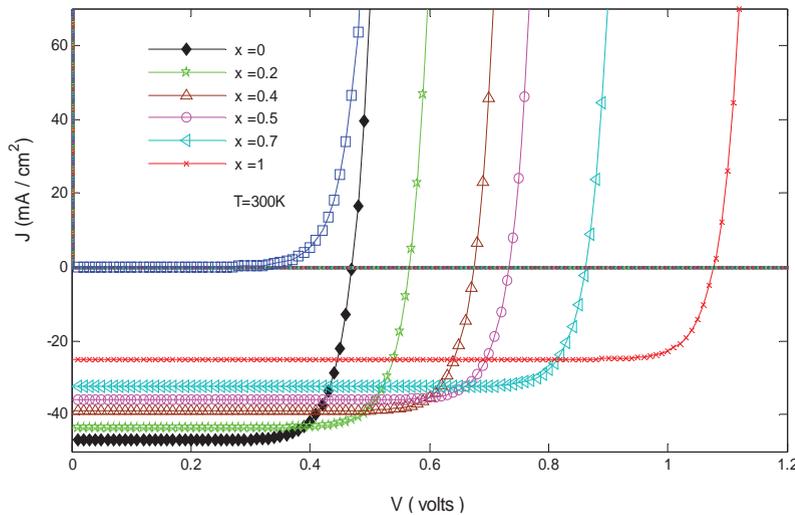


Fig. 5. J (V) characteristics of the $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$ structure for different composition (x)

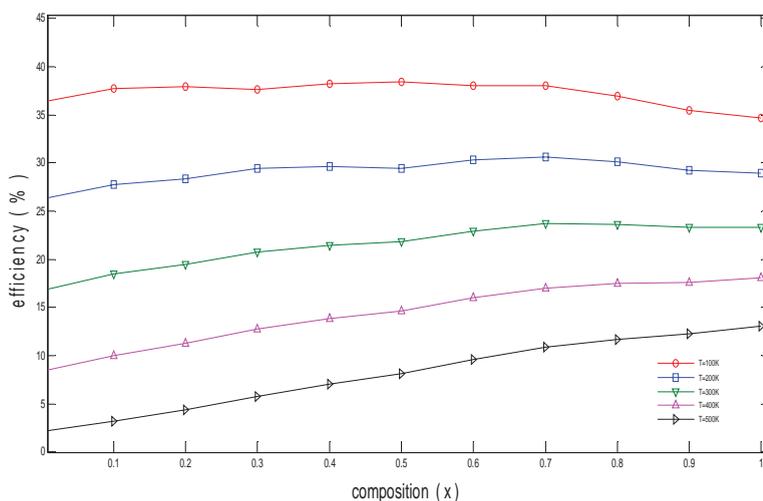


Fig. 6. efficiency variation versus the Gallium composition (x) at different temperatures (T)

4. Conclusion

In this work, we studied the main layers of solar cells based on the CIGS semiconductors. Then, we identified the influence of the composition of Gallium (Ga) on some physical and electrical properties (energy gap, lattice parameter, strain, absorption coefficient and the J (V) characteristic). We determined the evolution of efficiency according to the Gallium composition. Our study shows that the energy conversion efficiency η increases with the increasing of gallium composition. We noticed also that the increase in temperature reduces the efficiency η . For example, for a gallium composition $x = 20\%$ at a temperature of 300K we obtain $\eta = 19.47\%$. Meanwhile, the optimal conversion efficiency of 22% is obtained for $x = 50\%$ at $T = 300\text{K}$. For a temperature increase of 10 K (from 300 to 310K) which is equivalent to 10°C (from 27°C to 37°C) the efficiency decrease is only of 0.82%. This means that our designed solar cell structure made of $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$ semiconductor could be more reliable and temperature stable.

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