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Numerical Simulation of Tandem Using ZnS as a Buffer Layer Cu $I_{(1-x)}Ca_xSe_2/CuGaSe_2$

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Abstract

In the global context of diversification of usable energy sources, the use of renewable energies, in particular solar photovoltaic energy, is becoming increasingly important. As such, the development of a new generation of photovoltaic cells based on the CIGS material is promising. Indeed, the efficiency of these cells has exceeded 20% in recent years. Thus, our work consists in the modeling of a tandem solar cell based on $Cu(In,Ga)Se_2$ (CGS/CIGS). The goal is to optimize its physical and geometrical parameters in order to obtain a better photovoltaic conversion efficiency compared to other research works on tandem in the past. We used AMPS-1D software for the simulation. When we realize the tandem, the least efficient cell (CGS) imposes the current and the shape of the J-V characteristic of the tandem. We obtained a theoretical efficiency of 39.30% which is significantly higher than the efficiencies obtained in the past by other researchers with a short circuit current of 34.60 mA/cm^2, an open circuit voltage of 1.74 V and a form factor of 65.20%. The simulation also showed that the high defect density in the material strongly impacts the performance of the tandem.

Keywords

Photovoltaic Energy, Simulation, AMPS-1D, Tandem Solar Cell, Efficiency

1. Introduction

Energy has been the engine of human activity since antiquity, it plays a very important role in daily life and in the development of nations. According to the needs, several sources of energies are continuously developed related to the

progress of human civilization. Generally these energy sources are of fossil and fissile origin such as oil, natural gas, coal, uranium. Soaring costs and environmental pollution have led research to move towards so-called clean, renewable and inexhaustible sources on a human scale. The objective is to reduce our carbon footprint in all our domestic, agricultural and industrial activities and practices and also avoid waste in the exploitation and consumption of natural resources. All these precautions must be taken to preserve the planet and to reduce the share of negative impact that falls on the production of electrical energy. This requires a strong political will to stimulate, develop and promote renewable energies. The rulers have taken the right measure of what constitutes the threats and have committed themselves through the various Conferences of the parties on the climate (Cop). Researchers have emphasized research on clean and renewable energies. These depend only on regular natural phenomena mainly caused by the sun (thermal and photovoltaic solar energy, hydraulic, wind, biomass, …), the moon (tidal energy, certain currents: tidal energy, …) and the earth (geothermal energy). These energy sources are directly accessible locally, while fossil and fissile energies are only accessible in certain regions of the globe. Photovoltaics has already proven itself as a renewable energy source. Photovoltaic energy can be produced using a device called "Solar Cell" whose operation is based on "The Photovoltaic Effect". The solar cell is generally made from simple semiconductor materials (silicon, germanium) or compounds (gallium arsenide, cadmium telluride, etc.) which have well-adapted properties. Currently, silicon is the most widely used material for the manufacture of photovoltaic cells. It represents more than 80% of world production [1]. These silicon cells now occupy more than 90% of the photovoltaic market [2]. Although it holds a dominant place in the photovoltaic market, its maximum yield (25.60% in the laboratory) is very close to the theoretical limit of the maximum yield of 30% for a single junction [3] [4] with yields of 13% at 21% for marketed cells. Due to the manufacturing cost, competitive materials were investigated. Among these, mention may be made, for example, of semiconductors with a chalcopyrite structure, of the family of compounds I-III-VI2 based on CIS (Cu(In, Ga, Al)(Se, S)$_2$). Indeed, these compounds have bandwidths ranging from 1 eV ($CuInSe_2$) to 3 eV ($CuAlS_2$), which allows them to absorb most of the solar radiation. In addition, these materials are today those which make it possible to achieve the highest photovoltaic conversion efficiencies from thin-film devices [5], in particular Cu(In, Ga)Se_2 which is considered to be the most efficient, among all CIS-based derivatives [6]. Solar cells are currently the subject of much research with the aim of achieving the best ratio between energy efficiency and production cost. The fabrication of thin-film solar cells using Cu(In, Ga)Se_2, denoted (CIGS), represents a promising approach to reducing production costs.

The bandgap energy of Cu(In(1_x), Ga_x)Se_2 (CIGS) films varies in the range of 1.04 to 1.68 eV with the corresponding Ga content in CIGS films from $x = 0$ to 1 [7]. An increase in efficiency is expected mainly by using so-called tandem, triple and multi-junction solar cells, made of layers with different bandgap energies in

order to utilize different energy regions of the solar spectrum. The tandem solar cell consists of the upper high band gap cell, which absorbs the short wavelength (high energy) part of the spectrum, and the lower low band gap cell absorbing the rest. In this context, several researchers are trying to fabricate or simulate reliable tandem cells. In 2020, the CGS/CIGS double junction solar cell was simulated with and without gallium and its efficiency was 32.30% [8]. In 2021, work was carried out on double-junction perovskite structures with various compounds, including CIGS, which then led to an efficiency of 25%. Recently, an inorganic/organic perovskite tandem solar cell has been developed, whose Voc has been increased thanks to the SnO/ZnO electron transfer layer, with an efficiency of 20.18% [9]. Perovskite/CIGS and perovskite/Si double junction solar cells with 4-terminal architecture have been designed and tested, with reported efficiency of 25% and 25.70%, respectively [10]. In this work, we have opted for the modeling of a tandem solar cell based on Cu(In, Ga)Se_2 (CGS/CIGS). Indeed, numerical simulation makes it possible to avoid manufacturing several cell prototypes with different parameters, thus saving the time and cost of experimentation. It can also offer a physical explanation of the observed phenomenon since it allows the calculation of internal parameters such as recombination rates and free carrier densities. The aim of this work is to optimize the physical and geometrical parameters of the tandem solar cell based on Cu(In, Ga)Se_2 (CGS/CIGS) in order to obtain a better photovoltaic conversion efficiency compared to other tandem cell research in the past.

2. Materials and Methods

2.1. Numerical Simulation

A solar simulator is a set of programs based on digital discretization methods, allowing rapid modeling of semiconductor components. It is able to solve basic semiconductor equations such as Poisson equation and continuity equations of electrons and holes. It can also offer a physical explanation of the observed phenomena since they allow the calculation of internal parameters such as the recombination rate and the densities of free carriers. The use of AMPS 1-D is very practical because it makes it possible to simulate any photovoltaic structure and to go up to 30 layers. In addition, it allows the analysis of a wide range of device structures under illumination/under voltage or both, depending on the materials available in data files, by acting on the variable parameters (width, area, doping, etc.). A description Detailed resolution techniques can be found in the AMPS manual [11].

In this work, we used this software to, design the Cu tandem cell $I_{(1-x)}Ca_xSe_2$/$CuGaSe_2$. The parameters are to be introduced in three of the sub-windows constituting the main window of the AMPS 1-D software (**Figure 1**) [7].

In the sub-windows on the left, the working conditions are defined. These are the spectrum used, the temperature and the parameters of the front and rear contacts of the cell. The cell is illuminated when we activate the "light" box. In the sub-window located in the middle of the main window are introduced the

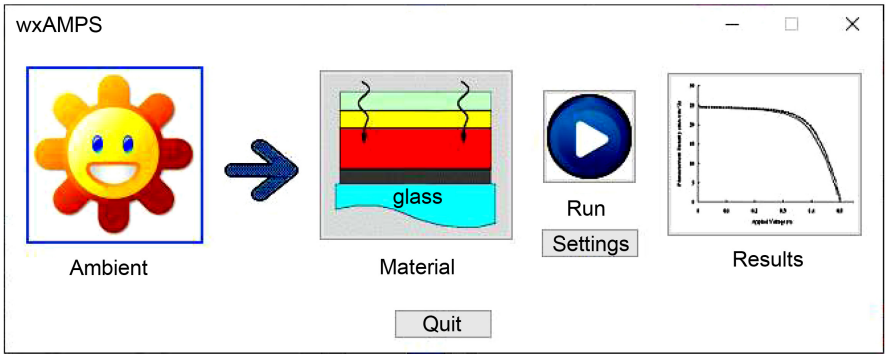

Figure 1. Main window of AMPS 1-D software.

structure of the cell and the parameters which define the spectrum of illumination. We find there the electrical characteristics, defects, geometrical and optical parameters. The thicknesses of the different layers are expressed in μm. In the sub-window on the right, the results of the simulation are indicated, *i.e.* the efficiency (η), the form factor (FF), the short-circuit current (J_{sc}) and the open-circuit voltage (V_{oc}).

2.2. CGS/CIGS Tandem Simulation Parameters

These are the physical and geometric parameters, in particular the electrical characteristics of the materials of the different layers (E_g, $\alpha(\lambda)$, N_C, N_V), their thicknesses and their dopings with the mobilities of the associated carriers. The cell is subjected to the global solar spectrum noted AM.1.5G with an incidence of 100 mW/cm^2 at 300 K. The reflection on the illuminated face is 5% while it is zero on the rear face. The material data was collected from the literature. They concern the concentration and mobility of the associated carriers, the electron affinity, the gap, the dielectric constant, the effective densities of states (N_C) and (N_V). The CdS buffer layer which is commonly encountered in the literature has been replaced by the ZnS layer. Table 1 gives the simulation parameters of the CGS/ CIGS tandem.

2.3. Determining the Form Factor and Efficiency

The form factor is the ratio between the maximum power supplied by the cell $P_{\max}$ and the product of the short-circuit current J_{sc} by the open-circuit voltage V_{co} (the maximum power of an ideal cell). It indicates the quality of the cell; It is of the order of 0.7 for efficient cells. It decreases with the rise in temperature and reflects the influence of losses by the two parasitic resistances R_s and R_{sh} [12].

It is determined using the relationship:

$$FF = \frac{J_{\max} V_{\max}}{J_{CC} V_{CC}} \tag{1}$$

The conversion efficiency of a cell is the quotient of the maximum power $P_{\max}$ by the incident power P_{in} (illuminance).

It results in the relationship:

Table 1. Simulation parameters of the CGS/CIGS tandem.

	p-CGS	n-ZnS	n-ZnO	p-CIGS	n-ZnS	n-ZnO
Epaisseurs (µm)	1	0.03	0.02	1	0.03	0.02
E_g (eV)	1.68	3.6	3.2	1.19	3.6	3.2
χ (eV)	4.5	4.15	4.5	4.5	4.15	4.5
e_r	13.6	9	9	13.6	9	9
N_C (cm^{-3})	6.8×10^{17}	2.2×10^{18}	3×10^{18}	6.8×10^{17}	2.2×10^{18}	3×10^{18}
N_V (cm^{-3})	1.5×10^{19}	1.8×10^{19}	1.7×10^{19}	1.5×10^{19}	1.8×10^{19}	1.7×10^{19}
μ_n (cm^2/Vs)	100	100	100	100	100	100
μ_p (cm^2/Vs)	50	25	31	50	25	31
Dopage (cm^{-3})	8×10^{16} (a)	10^{20} (d)	10^{19} (d)	2×10^{17} (a)	10^{20} (d)	10^{19} (d)

$$\eta(\%) = \frac{P_{\max}}{P_{in}} = \frac{FF \cdot J_{CC} \cdot V_{CO}}{P_{in}} \quad (2)$$

2.4. Structure of the CGS/CIGS Tandem Cell

The performance of a cell with one junction is limited due to the incomplete absorption of the solar spectrum (gap of the material used), the shading of the contacts of the illuminated face of the cell and the phenomena of radiative recombination in volume in quasi-neutral regions. To maximize the absorption of photons, we have opted for the simulation of a tandem cell in order to absorb high energy photons and low energy photons. **Figure 2** shows the structure of the CGS/CIGS tandem cell to be modelled. We will calculate the performance of the CGS/CIGS dual cell using AMPS-1D software, where the CGS ($x = 1$) is the forward cell and the CIGS ($x = 0.3$) cell [10] is placed backwards as shown in **Figure 2**.

3. Analysis and Interpretation of Simulation Results

3.1. Current-Voltage Characteristic Obtained after Simulation

The current-voltage characteristic of a dipole is the curve which translates the evolution of the voltage U at the terminals of the dipole according to the intensity J_{sc} of the current which crosses it. To obtain this curve, it is necessary to measure (J_{sc}) and U and to vary these parameters. **Figure 3** presents the characteristic current-voltage curve obtained after simulation of the CGS/CIGS tandem. We notice that from 0.10 to 0.80 V the curve remains constant for a value of $J = J_{CC} = 34.60$ mA/cm^2 and beyond 0.80 V it gradually decreases until it cancels out for $V = V_{OC} = 1.75$ V.

3.2. Yield and Form Factor of the CGS/CIGS Tandem Cell

The efficiency of solar cells depends on the number of junctions. In physics, the Shockley-Queisser limit also called the Shockley-Queisser efficiency limit relates to the maximum theoretical efficiency of a solar cell using a single PN junction to collect power from the cell [13]. The Shockley-Queisser efficiency limit puts

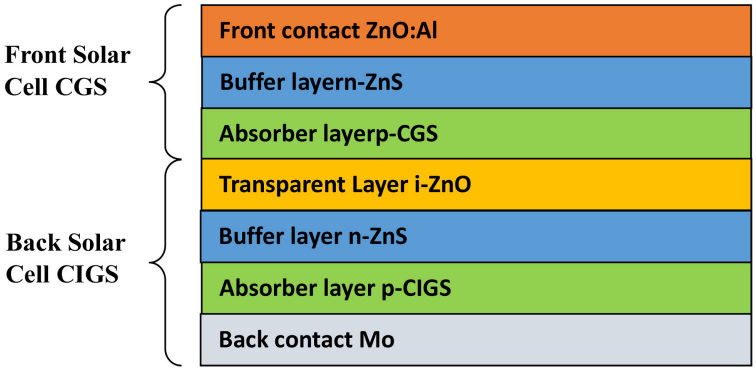

Figure 2. Schematic diagram of CGS/CIGS tandem solar cell.

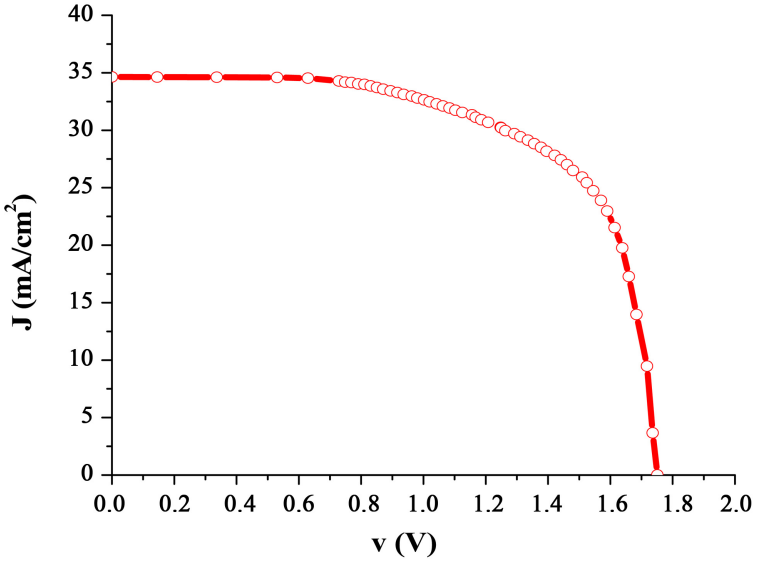

Figure 3. J-V characteristic of the CIGS/CGS tandem.

the maximum solar conversion efficiency around 33.70% assuming a single PN junction with a band gap of 1.34 eV (using an AM 1.5 solar spectrum). Modern commercial monocrystalline solar cells produce about 24% conversion efficiency, the losses largely due to practical concerns such as reflection from the front surface and light blocking of thin wires on its surface. The Shockley-Queisser limit only applies to cells with a single PN junction. Cells with multiple layers may exceed this limit. At the extreme, with an infinite number of layers, the corresponding limit is 86.80% using concentrated sunlight [14]. The curve in **Figure 4** translates the yield obtained during the simulation. It is 39.30%.

It indicates the quality of the cell; It is of the order of 0.70 for high-performance cells, it decreases with the rise in temperature. It translates the influence of the losses by the two parasitic resistances Rs and Rsh [3]. The curve in **Figure 5** is the graphical representation of the form factor obtained during the simulation. The resulting form factor is 65.20% or about 0.70, therefore very close to that of high-performance cells.

The photovoltaic parameters of the CGS/CIGS tandem cell extracted from this

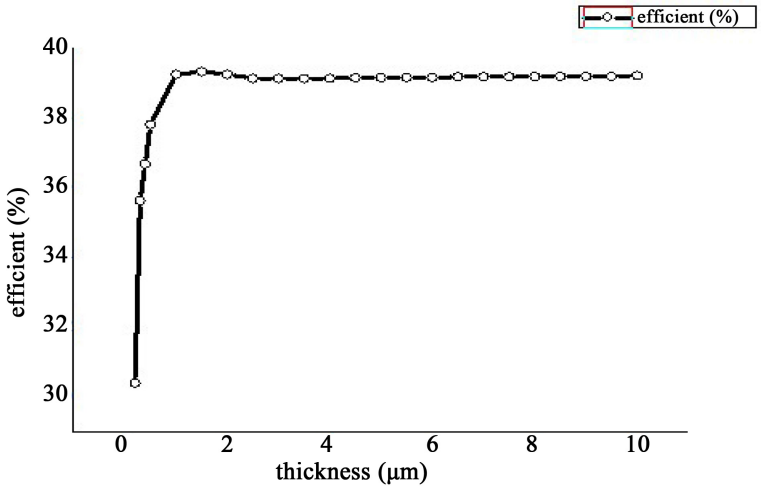

Figure 4. Yield of the CGS/CIGS tandem cell.

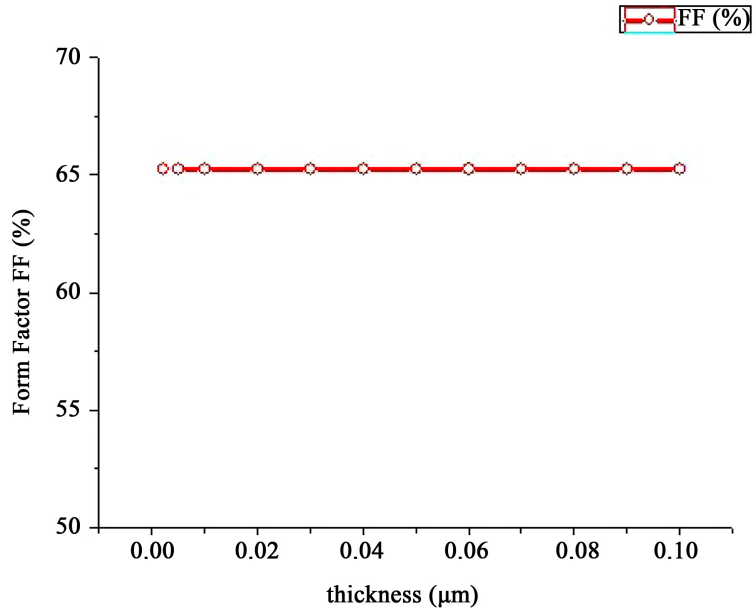

Figure 5. Form factor of the simulated CGS/CIGS tandem cell.

simulation are summarized in Table 2 and the resultant is given in Figure 6.

3.3. Comparison of the Photovoltaic Parameters of the CGS/CIGS Tandem Cell with Those of CGS and CIGS Single Junction Cells Encountered in the Literature

Table 3 shows the comparison of the CGS/CIGS tandem cell with the simulation results of CGS and CIGS single junction cells found in the literature. When we compare our results of the CGS/CIGS tandem cell with that found by other authors for a single CGS or CIGS cell, we can say that our results are better. The different J_{sc} encountered in the literature are 21.13 mA/cm^2 and 17 mA/cm^2 for CGS cells. Regarding CIGS cells, we have the values 36.42 mA/cm^2 and 35.17 mA/cm^2. The value of the tandem cell obtained after our simulation is 34.6

Table 2. Photovoltaic parameters from the simulation of the CGS/CIGS tandem cell.

V_{CO} (V)	J_{CC} (mA/cm²)	FF (%)	η (%)
1.74	34.60	65.20	39.30

Table 3. Photovoltaic parameters of the CGS/CIGS tandem cell and the CGS and CIGS single junction cells encountered in the literature.

cells	V_{CO} (V)	J_{CC} (mA/cm²)	FF (%)	η (%)	References
CGS cells	1.11	21.13	80.42	18.92	[15]
	1	17	74.03	16.42	[16]
CIGS cells	0.67	36.42	81.30	19.80	[17]
	0.73	35.17	83.54	21.31	[18]
CGS/CIGS tandem cell	**1.74**	**34.60**	**65.20**	**39.30**	Simulation results

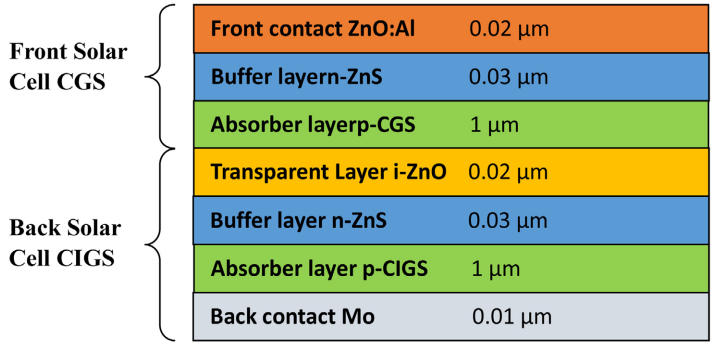

Figure 6. Schematic diagram of the CGS/CIGS tandem solar cell resulting from the simulation with the thicknesses of the different layers constituting it.

mA/cm². This value is close to and lower than those of single junction ones. This is because the J_{sc} of the tandem cell is limited by the low current of the lower CIGS cell. The open circuit voltage of the tandem cell which is 1.74 V is approximately equal to the sum of the open circuit voltages of the CGS and CIGS cells. The voltage V_{co} of the tandem cell is therefore the sum of the voltages of the cells based on CGS and CIGS. This equality confirms the law of the tensions of the compounds mounted in series. From these results, we can see the proper functioning of the CGS and CIGS cells connected in series forming the tandem cell. The value of the form factor resulting from the simulation, which is 0.65, is close to that of the high-performance cells, the value of which is 0.70. One can also notice an increase in the efficiency of the tandem cell compared to the cells produced separately. This improvement in efficiency is due to better absorption of solar radiation. The CGS cell absorbs high energy photons because of its higher gap (1.68 eV) and the lower gap CIGS cell (1.20 eV) absorbs long wavelengths.

Table 4. Table of the comparison of the photovoltaic parameters of the simulated CGS/CIGS tandem cell and those of tandem cells encountered in the literature.

Cells	V_{CO} (V)	J_{CC} (mA/cm^2)	FF (%)	η (%)	References
CIGS/CGS	1.7	17	82.41	25.14	[16]
perovskite/CIGS	2.25	25.80	73.02	30.71	[19]
CGS/CIGS tandem cell	**1.74**	**34.60**	**65.20**	**39.30**	Simulation results

3.4. Comparison of the Photovoltaic Parameters of the CGS/CIGS Tandem Cell Resulting from the Simulation with Those Encountered in the Literature

Table 4 presents the photovoltaic parameters of the simulated CGS/CIGS tandem cell and those of tandem cells found in the literature. The various simulation studies encountered have optimal conversion efficiencies of 25.14% [16] and 30.71% [19], while that of our simulation is 39.30%. This yield is clearly superior to other simulation results encountered in the literature. This improvement in the performance of the simulated tandem cell resulting from our work by other researchers is a considerable asset. The next challenge is the development of the prototype cell and the measurement of these photovoltaic parameters in order to validate our results.

4. Conclusion

In this work, we performed the simulation of a CGS/CIGS tandem cell. The AMPS-1D simulator was used to simulate the characteristics of the solar cell. An optimization of the photovoltaic parameters was made to have a good performance. Our simulation gave a theoretical yield of 39.30% which is significantly higher than the yields encountered in the literature. The short-circuit current is 34.6 mA/cm^2 with an open-circuit voltage of 1.74 V and a form factor of 65.20% which is very close to that of high-performance cells which are around 70%.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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