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Investigation of the ZnSe Layer, a Promising Buffer Layer Compared to the Reference CdS Buffer Layer

Daouda Oubda*, Boureima Ouédraogo, Sayouba Kabré, Alain Diasso, Soumaïla Ouédraogo, Marcel Bawindsom Kébré, Issaka Sankara, Boureima Traoré, Adama Zongo, Amidou Barry, Boureima Sawadogo, Pindéwindé Sawadogo, François Zougmoré

LA. M. E. (Laboratory of Materials and Environment), UFR-SEA (Training and Research Unit in Exact and Applied Sciences), Doctoral School of Sciences and Technologies Joseph KI-ZERBO University, Ouagadougou, Burkina Faso
Email: *daoudaoubd@gmail.com

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Abstract

In a context where access to electricity is a key issue to improve the satisfaction of the basic needs of populations, such as health, education, communication, etc., the need to find available, abundant energy production sources of energy is more than an obligation. This is why researchers in the field of renewable energies in general and in particular of photovoltaic solar energy (PV) investigate on different materials to considerably improve the stability and the conversion yield of PV solar cells. Therefore, in addition to the numerical simulation, we analytically simulate our photovoltaic (PV) solar cell model based on assumptions that simplify the basic equations. Thus, we simulate the opto-electrical parameters that we compare with those obtained from the numerical simulation. Our investigations show that the open-circuit voltage (V_{OC}) and the fill factor (FF) as a function of the thickness of the CIGS absorber simultaneous increase. Concerning the gap, we note an increase in FF for $1 < Eg < 1.3$ eV and a decrease for $Eg > 1.3$ eV and V_{OC} increases. The study carried out using alternative buffer layers shows good performances which are close to those of the standard buffer layer (CdS) and highlights the possibility of substituting the CdS buffer layer. The major advantage of these diapers comes from the fact that they are also non-toxic, the main raw material zinc is abundant and cheap. As for the space charge region (SCR), the study also shows good agreement between the numerical models and analytical models based on Equations (1) and (2). However, the analytical model presents a strategic issue which will allow us to further optimize the stability and opto-electrical performance of the CIGS-based solar cell using variables not accessible with the simulation software.

Keywords

PV Solar Energy, CIGS Solar Cell, Analytical Simulation, ZnSe Buffer Layer, Electrical Parameters

1. Introduction

In a context where access to electricity is a key issue to improve the satisfaction of the basic needs of populations such as health, education, communication, etc., the need to find available, abundant energy production sources of energy is more than an obligation. PV solar energy presents itself as a serious candidate to meet our needs. This is why researchers in the field of renewable energies in general and in particular of photovoltaic solar energy (PV) investigate on different materials to considerably improve the stability and the conversion yield of PV solar cells [1]-[4]. In addition to the experimental processes that are essential, the researchers have developed simulation software that optimizes the performance of PV solar cells, taking into account the physical, chemical, morphological and opto-electrical properties of different layers [3] [5].

The buffer layer plays an essential role in the operation of the photovoltaic (PV) solar cell in general and in particular the thin film heterojunction solar cell based on copper, indium, gallium and diselenide ($Cu(In,Ga)Se_2$). The use of the reference buffer layer, cadmium sulphide (CdS), made it possible to achieve historic record yields [6] but above all good operating stability [7].

Despite the good stability and record yields obtained with the use of the traditional buffer layer (CdS), the search for new buffer layers, called alternative buffer layers, is currently the ultimate objective of researchers in the PV field. The use of an alternative buffer layer should make it possible to avoid pollution due to the presence of cadmium (Cd), a toxic and carcinogenic element [8]. Several buffer layers are currently used in the experiment and in the simulation, we note among others: zinc selenide (ZnSe), sulfurous zinc oxide (Zn(O, S)) and zinc oxide and magnesium ((Zn, Mg)O) [9] [10]. Zinc-based buffer layers most often have a wide adjustable gap [11], moreover, the abundance of the main raw material zinc constitutes one of the most important characteristics of zinc-based layers. The interest of these alternative buffer layers in the PV field has been demonstrated by several works [12] [13].

ZnSe is part of the group of II-VI compounds, with a gap between 2.67 - 2.7 eV [14], ZnSe is a serious candidate for replacing CdS for the development of high-efficiency PV solar cells [14]-[16]. Interpretations suspect the formation of a thin layer of ZnS at the ZnSe layer/CIGS interface and would be very beneficial for the performance and stability of the PV solar cell [17].

In the remainder of our work, we will focus on all alternative buffer layers including the CdS reference buffer layer in general and in particular the zinc selenide (ZnSe) buffer layer. We first study the activation energy, then we study the electrical parameters of the different buffer layers by numerical simulation. Finally, we carry out a more in-depth study on the ZnSe buffer layer by numerically and analytically simulating the solar cell.

2. Materials and Methods

2.1. Structure and Operating Principle

The structure of the CIGS solar cell PV model that we simulate numerically and analytically, the role of each layer and the operating principle of the solar cell PV have been widely studied in our previous works [12] [18]-[20].

2.2. Numerical and Analytical Methods

Two simulation methods are available to us: the numerical method and the analytical method. The numerical method consists of using digital simulation software. We use the one-dimensional solar cell capacity simulation software (SCAPS-1D). The stability of this software for the simulation of solar cells based on Cu(In, Ga)Se_2 and the good agreement of the results obtained with this software in comparison with other simulation software were also addressed in our previous work [18]-[23].

The analytical model is obtained using assumptions simplifying the basic equations and allows us to calculate opto-electrical parameters which we compare with those obtained from numerical simulation with SCAPS-1D. The hypotheses (H) made are as follows [12]:

H1: AM1.5G illuminance is used for an ideal solar cell model, which allows us to ignore losses related to parasitic resistances (Rs and Rsh).

H2: the density of donors (Nd) in the p-type material and acceptors (Na) in the n-type material are neither negligible (low) nor high (too high) to ensure a highly effective electric field intensity in the SCR.

H3: High doping of the n-type material relative to the p-type material is considered, thus the SCR width is largely in the p-type material (CIGS), favoring the absorption of long-wavelength photons (900 nm ≤ λ ≤ 1200 nm) in or near the SCR. In addition, we obtain an acceptable SCR width that optimizes the electric field intensity, thus minimizing the recombination of photogenerated electron-hole pairs.

H4 (H6 becomes H4): Reflection is minimal at the front contact, allowing photons with wavelengths (300 nm ≤ λ ≤ 450 nm) to reach the p-n junction.

H5: (H4 becomes H5) We consider a p-n junction width of 1030 nm, *i.e.*, W (n) = 30 nm and W (p) = 1000 nm. This p-n junction width is intended to develop a stable, lightweight and highly efficient PV solar cell design. The wavelength λ varies between 300 and 1200 nm, allowing us to account for the contribution of high-energy, short-wavelength photons.

H6 (H5 becomes H6): only absorptions in the CdS/ZnSe buffer and the CIGS absorber layers are considered.

H7: In the absence of optical excitation, there is no mobile charge carrier (electrons and holes) in n and p-type materials. The current density contribution of the electrons and mobile holes is zero.

The simplified expressions for the current density of electrons and that of holes are given respectively by Equations (1) and (2).

$$J_n = -qD_n \frac{dn_p}{dx} \quad (1)$$

$$J_p = -qD_p \frac{dp_n}{dx} \quad (2)$$

These equations are solved analytically by applying the initial and boundary conditions of contacts [24].

Table 1 summarizes the parameters of the different buffer layers studied.

Table 1. Bases parameters of CIGS cell properties. W—thickness, ε—dielectric constant, E_g—band gap energy, ΔEC—conduction band offset, σ_e, σ_h—capture cross section electrons and holes, χ_e—electron affinity, υ—thermal velocity, N_a, N_d—shallow uniform acceptor and donor density.

Layer Properties					
	p-CIGS	n-CdS	n-ZnSe	n-Zn(S,O)	n-(Zn,Mg)O
W [nm]	500 - 3000	30	30	30	30
Eg [eV]	1 - 1.6	2.4	2.67	3.3 - 3.6	3.3 - 3.9
χ_e [eV]	4.5	4.45	4.44	4.38	4.34
$\varepsilon/\varepsilon_0$	13.6	10	9.1	9	9
N_c [cm^{-3}]	$2.2 * 10^{18}$	$2.2 * 10^{18}$	$2.2 * 10^{18}$	$2.2 * 10^{18}$	$2.2 * 10^{18}$
N_v [cm^{-3}]	$1.8 * 10^{19}$	$1.8 * 10^{19}$	$1.8 * 10^{19}$	$1.8 * 10^{19}$	$1.8 * 10^{19}$
ve [cm/s]	$5 * 10^6$	10^7	10^6	10^6	10^6
vh [cm/s]	$5 * 10^6$	10^7	10^6	10^6	10^6
μe [cm^2/Vs]	10^2	10^2	10^2	10^2	10^2
μh [cm^2/Vs]	25	25	25	25	25
N_a [cm^{-3}]	$2.5 * 10^{16}$	-	-	-	-
N_d [cm^{-3}]	-	$2.5*10^{16}$	10^{17} [D]	10^{17} [D]	10^{17} [D]

3. Results and Discussions

3.1. Numerical Method

3.1.1. Electrical Parameters as a Function of the Simultaneous Variation of the Thickness and the Gap of the CIGS Absorber

In this section, we investigate the evolution of the open-circuit voltage (V_{OC}) and the form factor (FF) as a function of two very sensitive parameters in the operation of solar cells and very important for performance optimization. This is the thickness and the gap of the CIGS absorber. Figure 1 and Figure 2 show the results obtained with SCAPS-1D for different buffer layers.

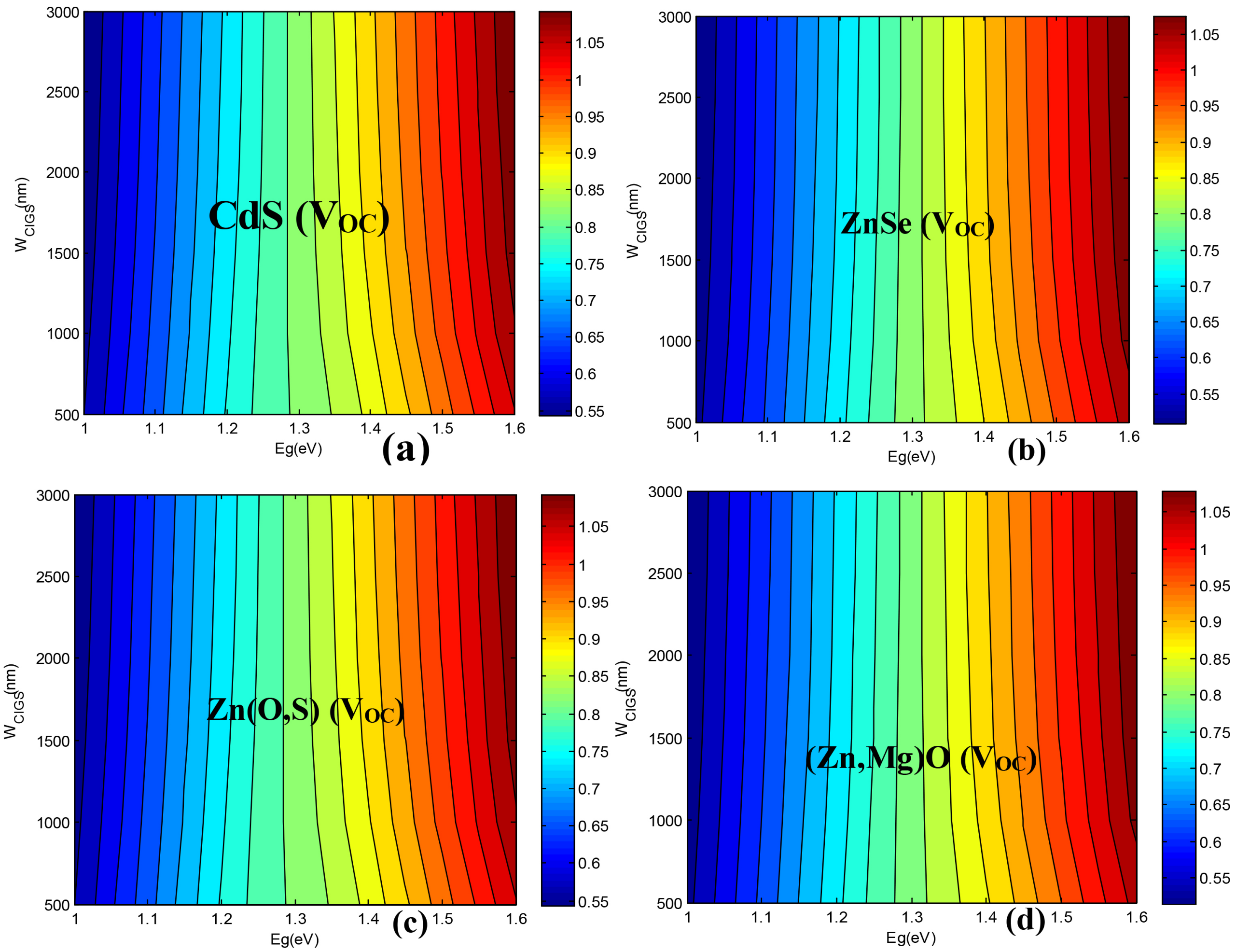

Figure 1. Evolution of the V_{OC} as a function of the thickness and gap of the CIGS.

We see almost similar evolutions of the curves of the different alternative buffer layers. The electrical parameters of the solar cell with CdS buffer layer have an evolution which differs little from those of alternative buffer layers. This may explain the stability exhibited by CdS buffer layer solar cells. Our investigations show that the open-circuit voltage (V_{OC}) and the fill factor (FF) as a function of the thickness of the CIGS absorber simultaneously increase (Figure 1, Figure 2). Concerning the gap, we note an increase in FF for 1 < Eg < 1.3 eV and a decrease for Eg > 1.3 eV) and V_{OC} increases (Figure 1, Figure 2). These results obtained on the alternative buffer layers are satisfactory and encouraging. The major advantage of these diapers comes from the fact that they are also non-toxic. In addition, the main raw material Zinc is abundant and cheap.

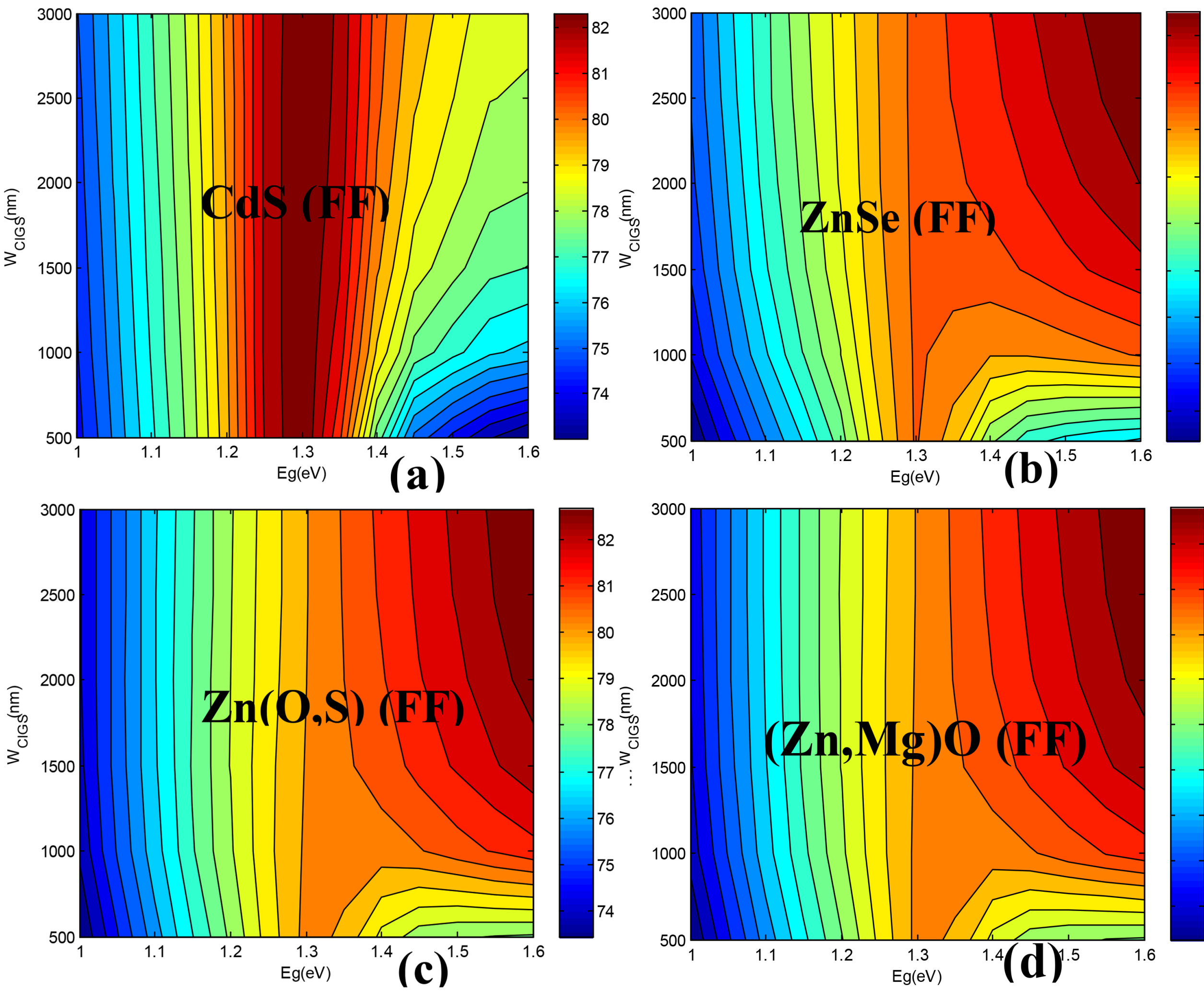

Figure 2. Evolution of the FF as a function of the thickness and the gap of the CIGS.

3.1.2. Activation Energy of Alternative Buffer Layers

In this section, we determine the activation energy of the CIGS solar cell with CdS buffer layer by extrapolation of the V_{OC} graph as a function of temperature according to the method presented in [25] [26]. The method of the determination consists to plot the V_{OC} curve as a function of temperature and we use the following relation (Equation (3)):

$$V_{OC} \approx \frac{E_a}{q} - \frac{kT}{q}\ln\left(\frac{I_{ph}}{I_0}\right) \quad (3)$$

We graphically obtain the activation energy by extrapolating the curve up to the temperature of $0K$ at the origin of the benchmark $\left(\frac{kT}{q}\ln\left(\frac{I_{ph}}{I_0}\right) \approx 0\right)$. The value of the V_{OC} read corresponds to the value of the activation energy to a factor of $1/q$ ($V_{OC} = E_a/q$).

The objective in this part is to determine by the same procedure the activation energy of each alternative buffer layer. The results obtained can be observed in the figure (**Figure 3**).

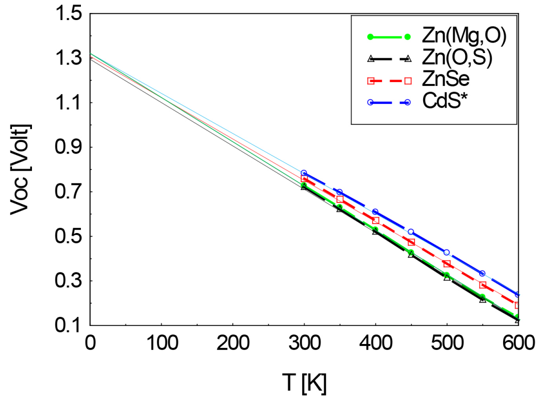

Figure 3. Determination of the activation energy of alternative buffer layers.

The value of the activation energy of all the alternative buffer layers is approximately equal to 1.3 eV (Ea ≈ 1.3 eV) which is that of the reference buffer layer (CdS) (**Figure 3**). The study carried out using the alternative buffer layers in addition, to the good performances shows a better stability which are close to those of the standard buffer layer (CdS) and highlights the possibility of substituting the CdS layer.

3.2. Analytical Method

3.2.1. Characteristics of Current-Voltage Densities and Quantum Efficiency

Figure 4 presents the curves of the J-V characteristics and quantum efficiency obtained from the numerical and analytical models. We observe good profile agreement for the J-V characteristic with a slight overestimation by the analytical method. As for the quantum yield, the analytical model is representative for wavelengths beyond 500 nm and gives good agreement. Thus, the analytical model makes it possible to complete the software to assess the performance of a CIGS/ZnSe solar cell based on certain variables.

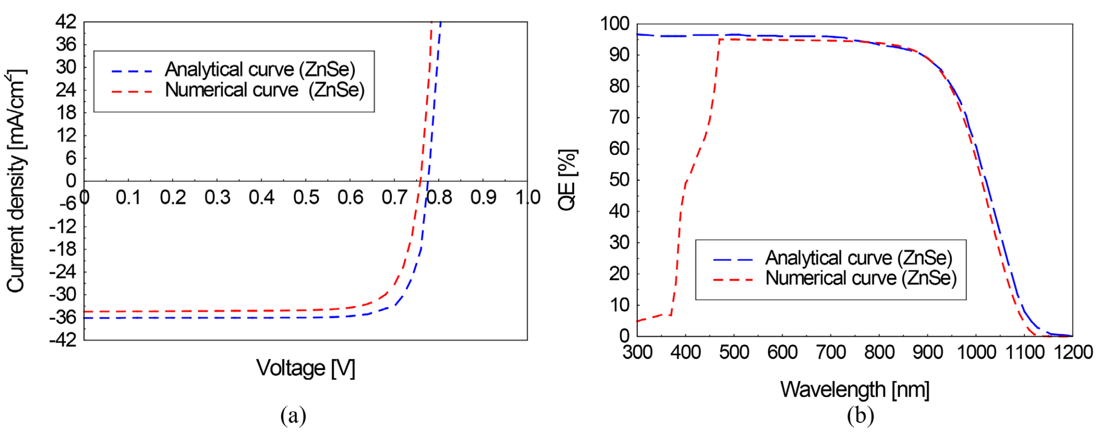

Figure 4. Curves of the characteristics of (a) voltage current density and (b) quantum efficiency.

3.2.2. Electrical Parameters Depending on the Width of the Space Charge Region (SCR)

In this part, we have chosen to analytically simulate the ZnSe-based solar cell with a new variable of capital importance because it is very sensitive to stability and optimization of performance. Given that the majority of electron-hole pairs are generated inside the SCR and that their recombination leads to a significant reduction in the values of all the electrical parameters and more particularly the conversion efficiency, it is interesting to work at short and long term to be able to obtain an optimal width of the SCR which minimizes the recombination of charge carriers.

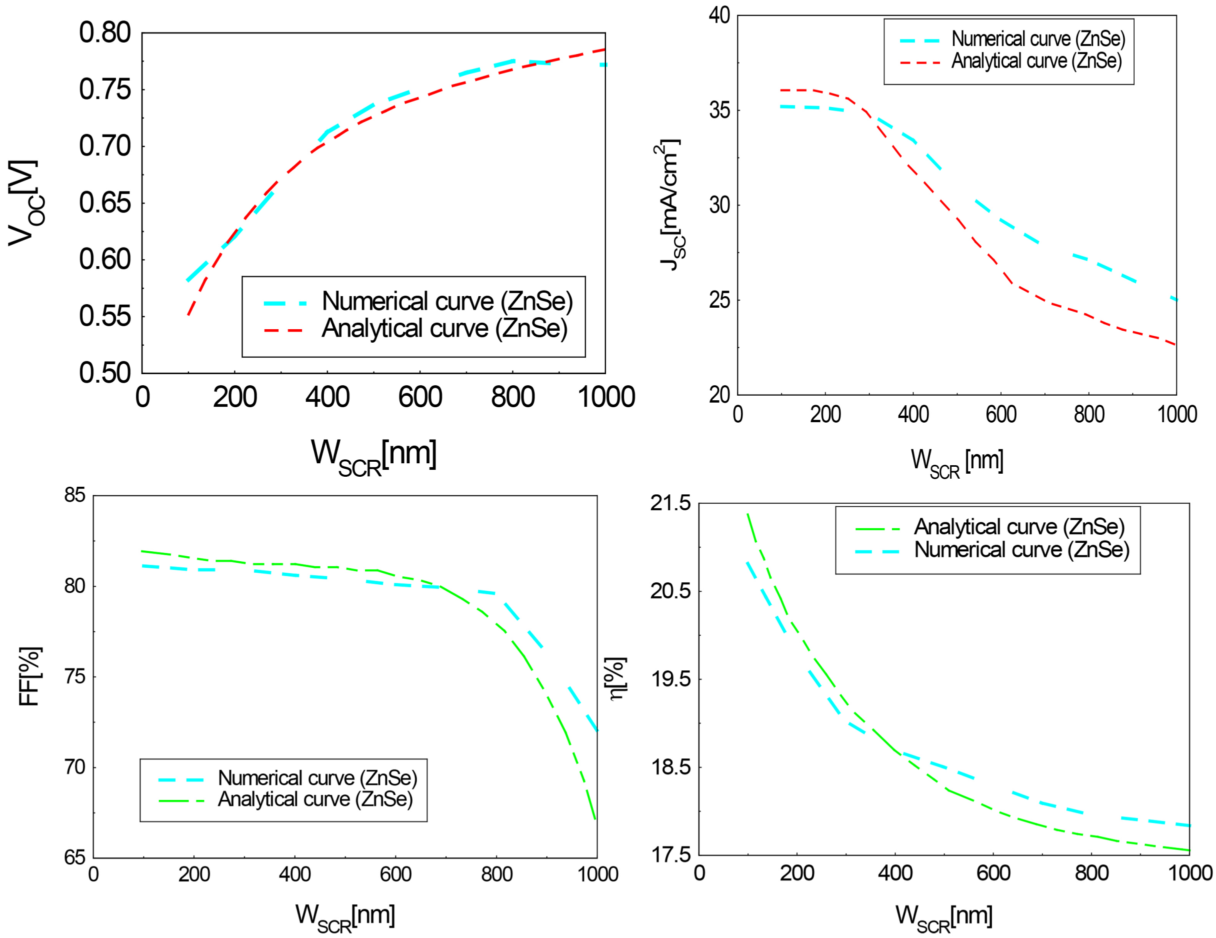

Figure 5. Electrical parameters depending on the width of the ZCE.

The compared curves of the electrical parameters (Voc, Jsc, FF, η) in **Figure 5** show good agreement between the numerical models with SCAPS-1D and the analytical models from Equations 1 and 2. The analytical model, which is simplistic and derives from simplifying hypotheses, makes it possible to properly assess the behavior of the CIGS solar cell. The advantage of the analytical model is that it makes it possible to obtain variations in the opto-electrical parameters of the solar cell using variables that cannot be accessed with simulation software.

4. Conclusions

In this article, the study of the chalcopyrite thin-film solar cell based on the quaternary CIGS system was carried out using the digital simulation software SCAPS-1D but also using an analytical method. The results of the numerical simulation show that the evolution of the curves obtained with the CdS buffer layer presents a slight difference and which explains its good stability. It also appears on the one hand that the simultaneous increase in the thickness and the gap of the absorber leads to an increase in V_{OC}, and in the FF for $1 < Eg < 1.3$ eV. On the other hand, we find a value of the activation energy of all the buffer layers approximately equal to 1.3 eV and highlight the possibility of substitution of the CdS layer, in this case, it is verry important to precise that the solar cell with CdS buffer layer and ZnSe buffer layer presents electrical parameters that are sensibly equal. For CdS buffer layer we have: $V_{OC} = 0.78$V, $J_{SC} = 34.30$ mA/cm^2, FF = 79.80%, $\eta = 21.42\%$ and for ZnSe buffer layer we have: $J_{SC} = 34.6$ mA/cm^2, $V_{OC} = 0.76$ V and FF = 79.6%, $\eta = 20.76\%$.

As for the space charge region (SCR), the study also shows good agreement between the numerical models with SCAPS-1D and analytical models based on Equations (1) and (2). However, the analytical model presents a strategic issue which will allow us to further optimize the stability and opto-electrical performance of the CIGS-based solar cell using variables not accessible to the simulation software.

Conflicts of Interest

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

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