Chalcogenide Letters Vol. 18, No. 8, August 2021, p. 457 - 465

Theoretical simulation of ZnS buffer layer thin films with SCAPS-1D software for photovoltaic applications

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This Work represents the influence of some parameters (Temperature, existence of Buffer layer and its thickness), using a Numerical simulation of thin film solar cells, named SCAPS (which is a one-dimensional solar cell capacitance simulator) in modeling of the high efficiency CIGS-based solar cells (with efficiency of η=10.87%).In each case, the photovoltaic parameters have been calculated. It has been concluded that, the efficiency of CIGS-based solar cells is decreasing with increasing of the temperature and the thickness of Zinc Sulfide buffer layer. However, when the buffer layer doesn't exist in solar cells photovoltaic, we noticed that the efficiency of solar cells is increasing to (η=12.04%) under the AM1.5 spectrum, one sun and at room temperature, with increasing of the short-circuit current density (Jsc), and decreasing of open-circuit voltage (Vco).

(Received April 27, 2021; Accepted August 10, 2021)

Keywords: SCAPS, Open circuit voltage, Short current density, Solar cell, Modelling

1. Introduction

The Solar cell thin film based on CIGS is a 1-II-V_2 semiconductor material composed of copper, indium, gallium, and selenium. It had proved him role on terrestrial applications thanks to their high efficiency, long-term stable performance and potential for low-cost production. In fact, this typical solar cells polycrystalline provide a good alternative to wafer based crystalline silicon solar cells, which currently constitute the major share of photovoltaics installed and used worldwide. [10-11] (in our case, we will study the CIGS-based solar cells wich the efficiency is 10.87%). Normally, the band gap of these semi-conductor is direct which minimize the requirement for long minority carrier diffusion lengths [2-10-11].However, Cadmium is a metal that can cause severe toxicity in humans and the environment [3]. For this reason, we decide to replace this dangerous material by Zinc (Zn) and we present a numerical study of the thin film CIGS-based solar cells with SCAPS, wich is used to calculate the photovoltaic parameters at sunder standard illumination (AM1.5G, 100 mW/cm^2,300K). We studied also the influence of: Temperature, existence of buffer layer and the effect of its thickness on the performance of the CIGS-based solar cells. The J-V characteristic has been calculated to get the optimal value of efficiency, without using CdS.

1.1. Literature overview

CIG-based thin film solar cell started to receive even more attention in 1981 when Mickelsen and Chen achieved an efficiency of 9.4% by using co-evaporation technique from elemental sources [13]. From that onwards, numbers of emerged technologies such as alloying CIS with gallium (Ga) to become Copper Indium Gallium Selenide (CIGS), incorporating sodium (Na) into the CIGS absorber layer, and replacing thick cadmium sulfide (CdS) buffer layer with thin CdS layer have boosted the efficiency significantly. Copper Indium Gallium Selenide (CIGS) thin film solar cell currently holds a record efficiency of 22.6% since 2016 [14].The cell structure of CIGS is known as substrate configuration where the light enters the cell through Transparent Conducting Oxide (TCO), passes through the buffer layer, is absorbed by the CIGS, and then reaches the back contact, usually molybdenum, which is deposited on the substrate. The reason CIGS has been one of the most promising absorber layer for thin film photovoltaic devices is due to its high absorption coefficient for solar radiation and compatibility of its band gap (1.6 eV–1.0 eV) [15].The advantages

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https://doi.org/10.15251/CL.2021.188.457

of CIGS-based solar cells over CIS-based solar cells are as follows: (i) the band gap can be tuned by adjusting the Ga/In ratio to match the solar spectrum. If all indium (In) is replaced by gallium (Ga), the CIGS band gap increases from about 1.04 eV to 1.68 eV [16]. It has been stated that CIGS absorber layer can absorb most parts of the solar spectrum with a thickness of 1 μm [17]. Hence, a layer thickness of ~2.0–2.5 μm will be sufficient for the completed device, and a thinner layer device means reduction in raw material usage and lower production cost incurred. (ii) Ga incorporation can also improve the open-circuit voltage V_{oc} of CIGS since V_{oc}~$E_g/2$ (E_g is referring to band gap) [17]. Moreover, CIGS thin film solar cell has very high potential to overcome the cost level of conventional PV crystalline silicon (c-Si) technology [10]. The c-Si modules with efficiencies of 19–23% will have a production cost of $0.6–$0.7/Wp [18]. Whereas for CIGS modules, manufacturing cost of $0.75/Wp can be achieved at 50 MW/yr production capacity with an average efficiency of 12% [19]. The substrate in CIGS has a crucial role in the development of the whole device. Deposition of the molybdenum back contact on rigid or flexible substrate will define the selenization condition.

1.2. Motivations and aim of study

The following layer in CIGS after substrate is the molybdenum (Mo) back contact which acts as an optical reflector to reflect the light back to the absorber layer in CIGS solar cell [1,2]. Molybdenum (Mo) is a preferred back contact material for CIGS solar cells because it does not react strongly with CIGS; it forms low-resistivity ohmic contact to CIGS, and the conductivity of Mo does not degrade during deposition of CIGS at high substrate temperature [3,4]. Mo has high conductivity and is more chemically stable and mechanically stable during CIGS growth (selenization) than other materials such as W, Ta, Nb, Cr, V, Ti, and Mn [5,6].The layer after Mo back contact is Copper Indium Gallium (CIG) before going through the process of selenization. During the selenization process, selenium (Se) vapor will react with CIG to become CIGS and react with Mo to form the $MoSe_2$ layer. This interfacial layer between Mo and CIGS is beneficial in terms of having a wider band gap (1.35–1.41 eV) than CIGS, hence it can absorb more near-infrared light to improve the cell performance [7]. The formation of $MoSe_2$ layer does not depend only on the selenization condition but also on the properties of the Mo film [8, 9]. Therefore, improving the properties of the Mo film can promote the growth of $MoSe_2$ layer. Recently, substrates used in CIGS, either rigid or flexible, together with the properties of the Mo back contact and the $MoSe_2$ interface layer were discussed in various papers [10,11,12]. This paper aims to focus on the mentioned area by first providing an overview of comparison between conventional PV and thin film solar cells followed by reporting the recent progress of the substrates in CIGS, specifically regarding the available substrates. This paper will then converge towards the Mo layer in CIGS and further discuss about the deposition techniques and effect of deposition condition on the properties of Mo back contact. Then, the formation and thickness influence factors of the interfacial $MoSe_2$ layer will be reviewed in this paper. Scale-up issues of CIGS module production will also be presented to give an insight into commercializing CIGS solar cells.

2. Numerical Modeling of SCAPS-1D Software

The structure of the CIGS forms a complex junction made of materials of different types (heterojunction) of CIGS (p) / CdS (n) / ZnO (n) type in the higher efficiency devices. In this structure, CIGS is a p-type wide-band gap absorber layer, wich is deposited on the molybdenum coated back glass substrate. the other members of this junction is a buffer layer n-type (Zinc Sulfied thin films) and a window layer n-type (ZnO) (figure 1).The OVC layer is considered to be beneficial to the performance of CIGS cells because the electrical junction is shifted away from the high-recombination interface between the CdS and CIGS layer, and hence, the recombination rate is reduced [13]. The TCO is covered with an antireflection layer MgF_2, which increases the absorption of photons in the absorber layer.

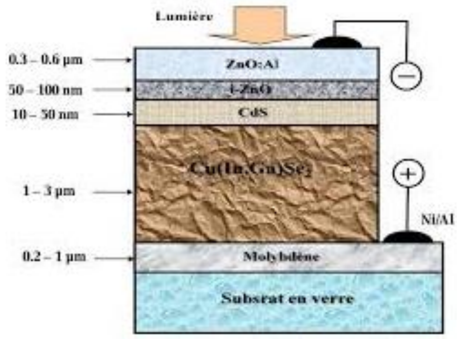

Fig. 1. Schematic cross-section of CIGS based solar cells.

In this paper, we will study some parameter optimization of solar cells, using SCAPS-1d software. It is a one dimensional solar cell simulation program developed at the department of Electronics and Information Systems (ELIS) of the University of Gent, Belgium. Several researchers have contributed to it's development: Alex Niemegeers, Marc Burgelman, Koen Decock, Johan Verschraegen, Stefaan Degrave. A description of the program, and the algorithms it uses, is found in the literature [20-25].In first, we start by define the problem, on clicking on set problem, than we define the working point by specifing the parameters which are not varied in a measurement simulation, and which are relevant to that measurement, than we select the measurement (s) to simulate (I-V); (C-V); C- and Q(E)(λ) [20-25]. Finally, we start the simulation by clicking button Calculate Single shot.

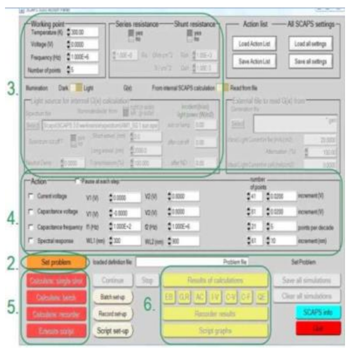

Fig.2.The SCAPS start-up panel: the Action panel or main panel.

1.Run SCAPS;

2.Define the problem, thus the geometry, the materials, all properties of your solar cell;

3.Indicate the circumstances in which you want to do the simulation, i.e. specify the working point;

4.Indicate what you will calculate, i.e. which measurement you will simulate;

5.Start the calculation(s);

6.Display the simulated curves.

Table 1. Parameters set for CIGS solar basics cells at room temperature (300 k) and at A.M 1,5 G.

Parameters	i-ZnO	OVC	CdS	CIGS
Thickness (μm)	0.080	0.015	0.100	1.000
Band Gap (eV)	3.400	1.450	2.450	1.200
Electron affinity (eV)	4.550	4.500	4.450	4.500
Dielectric permittivity (relative)	10.000	10.000	10.000	10.000
CB effective density of stattes (cm^{-3})	4.000E+18	2.000E+18	2.000E+18	2.000E+18
VB effective density of states (cm^{-3})	9.000E+18	2.000E+18	1.500E+18	2.000E+18
Electron thermal velocity (cm/S)	1.000E+7	1.000E+7	1.000E+7	1.000E+7
Hole thermal velocity (cm/S)	1.000E+7	1.000E+7	1.000E+7	1.000E+7
eLectron mobility (cm^2/V.S)	5.000E+1	1.000E+0	5.000E+1	5.000E+1
Hole mobility (cm^2/V.S)	2.000E+1	1.000E+0	2.000E+1	2.000E+1

3. Results and discussion

3.1. Impact of buffer layer thin film:

The buffer layer is a thin film located between the absorbent layer and the layer transparent conductive oxide (TCO). Its role is to be as much transparent as possible, allowing a maximum sunlight absorption in the absorber layer while maintaining a low interface recombination rate [12]. When the transparent conductive oxide layer (TCO) and the absorbent layer (CIGS) are directly putting in contact, we may get in this case a photovoltaic junction, but its performance will be limited by the unsuitability of band gaps and existence of short-circuits density.It has benne proved that without buffer layer thin films in CIGS based solar cells, the efficiency is increasing (from 10.84% to 12.04%) with increasing of density short circuit (from 31.68649 mA/cm^2 to 33.30812 mA/cm2) and with decreasing of open circuit voltage (from 0.5587 v to 0.5542 v). In fact, Buffer layer optimizes the alignment of the bands between the CIGS and the window layer and to limit the recombination carriers at the interface of these two layers. It also assures, the protection of the surface absorber during sputter deposition of the ZnO layer, wich can be caused the formation of defects on the CIGS surface layer.

Table 2. Impact of buffer layer thin film on CIGS solar cells.

Parameters	Voc	Jsc (mA/cm2)	FF (%)	Efficiency(%)
With buffer layer	0.5587	31.68649	61.40	10.84
Without buffer layer	0.55420	33.30812	65.24	12.04

3.2. Impact of ZnS buffer layer thickness on solar cells performance:

In this part of the simulation, we started by choosing the thickness of CIGS layer set to 1 µm, and we changed the thickness of Zinc Sulfied (ZnS) buffer layer, from 20 nm to 300 nm. We noticed, that the high efficiency is decreasing with the increasing of the thickness of ZnS buffer layer. We noticed also, that the high efficiency of CIGS film solar cells is decreasing with the increasing of Zinc Sulfied buffer layer thickness (from 11.88% for 20 nm to 5.13% for 300 nm). When the buffer layer thickness increase, a large number of short wavelength photons are absorbed in this layer before reaching the absorber layer. This lead to a decrease in the photons which have reached the absorber layer. Moreover, the minority carriers of the CdS buffer layer (holes) have a lower mobility compared to that of CIGS absorber layer (electrons)Hence the decrease in the cell performance [30]. It has a an influence on elecrtical properties, because it creats he electric field results of the junction within of space charge region. Figure shows the variation of buffer layer thickness (ZnS) on the performance of CIGS based solar cells:

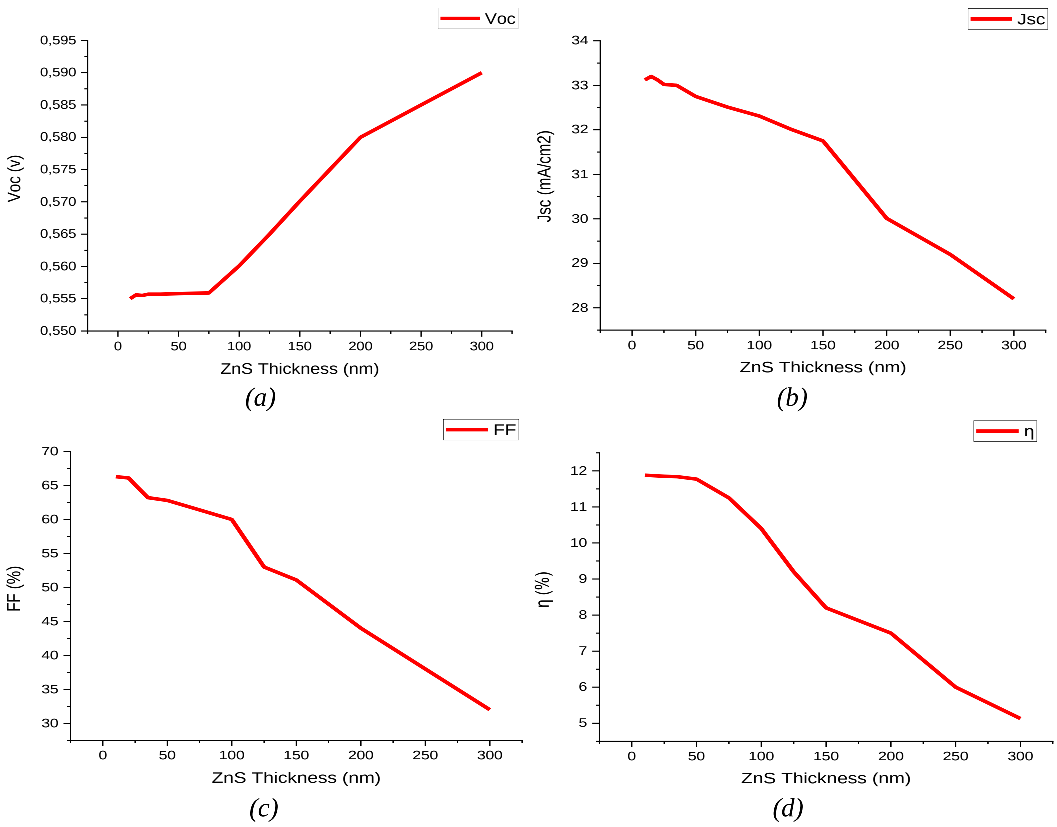

Fig.3.The Effect of ZnS buffer layer thickness on the CIGS films solar cells performance: 3a (Open circuit voltage), 3b (schort current density), 3c (Fill Form), 3d (Efficiency).

3.3. Impact of temperature, on the CIGS-based solar cells, using CdS as buffer layer

One of the most parameter optimization in solar cells thin films is the operating temperature, wich acts an important role in the examination of the performance of solar cells thin films. We studied here the influence of high Temperature on the Solar cells performance of CIGS and we have evaluated effect of temperature on the performance of thin film CIGS-Based solar cells. As we can see, the performance of the solar cells thin films is decreasing with the increasing of the higher operating temperature.

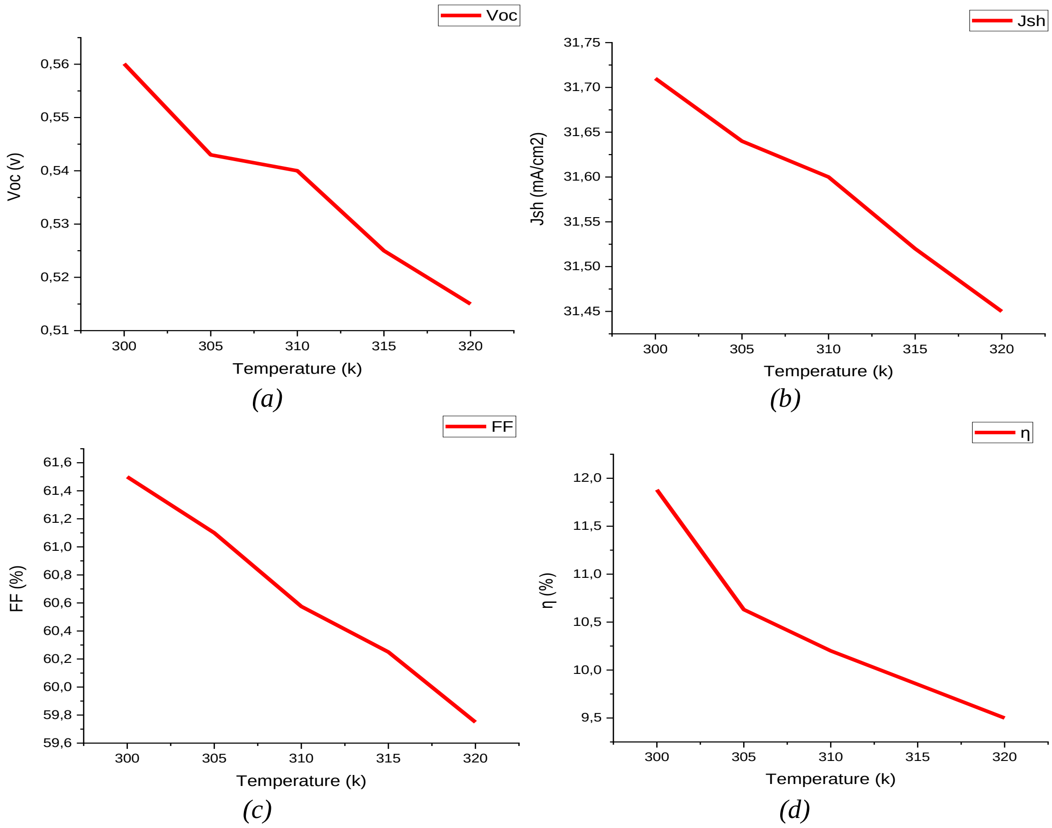

Fig.4.The Effect of Temperature on CIGS films solar cells performance using CdS as buffer layer: 4a (Open circuit voltage), 4b (schort current density), 4c (Fill Form), 4d (Efficiency).

3.4. Impact of temperature, on the CIGS-based solar cells, using ZnS as buffer layer

The Goal of replacement of the CdS Buffer layer by ZnS buffer layer, here, is optimizing the variation of all solar cells properties, to see, wich material would be the performant one, that can be explained mathematically, by the values of variation of these characteristics. In first, we study the influence of the temperature on CIGS-based solar cells, using ZnS as Buffer layer. Under AM1.5Gillumination spectra, it has been seen that with increasing temperature, increases, and thus, Short current density decreases. And therefore, the fill factor and the efficiency of the cell also decrease. This explains that ZnS will be a good alternatif material to replace CdS in photovoltaic applications. The Fig. 5 shows the influence of operating temperature on CISG based solar cells, using ZnS as buffer layer.

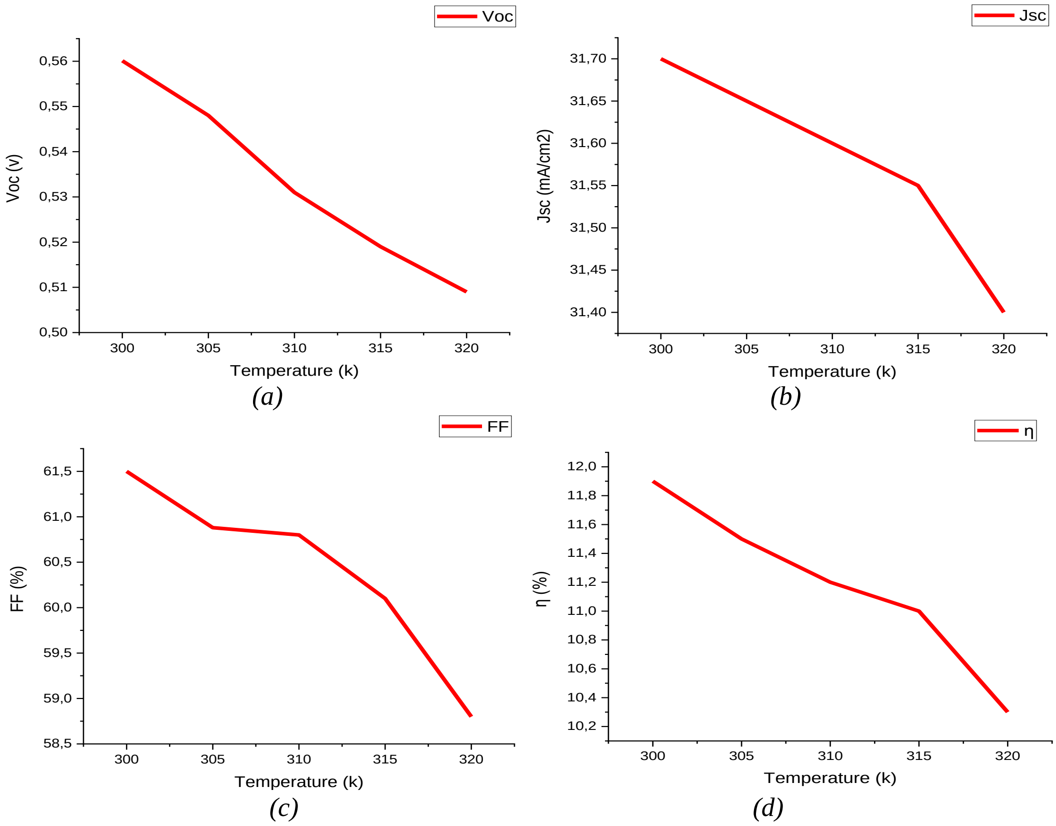

Fig.5. Effect of the Temperature on performance of solar cells, using ZnS as Buffer layer: 4a (Open circuit voltage), 4b (schort current density), 4c (Fill Form), 4d (Efficiency).

3.5. Comparaison between the efficiency of solar cells using ZnS and CdS as buffer layers

We can notice, that the performance of CIGS-Based solar cells (Efficiency, Open circuit Voltage, Short current density and fill form), is decreasing with increasing of the Temperature. We made in this part of the paper a comparison, in order to optimize the rate of variation of the solar cells efficiency, to make sure if our material (ZnS) is challenger to Sulfied Cadmium (CdS):

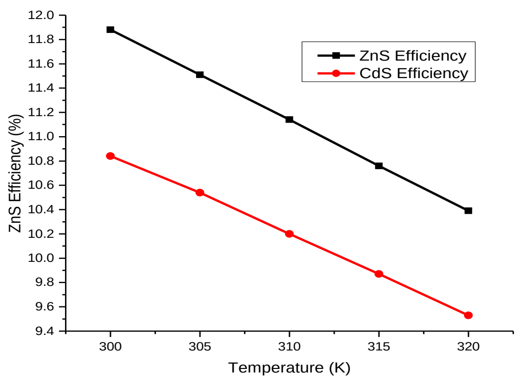

Fig.7. The effect of temperature in the efficiency of Zinc Sulfied and Cadmium Sulfied buffer Buffer layer.

We can notice also, that the Zinc Sulfied buffer layer thin film and Cadmium Sulfied buffer layer thin films have the same curve, it tells as that with the presence of high temperature, Zinc Sulfied buffer layer can replace the Cadmium sulfide.

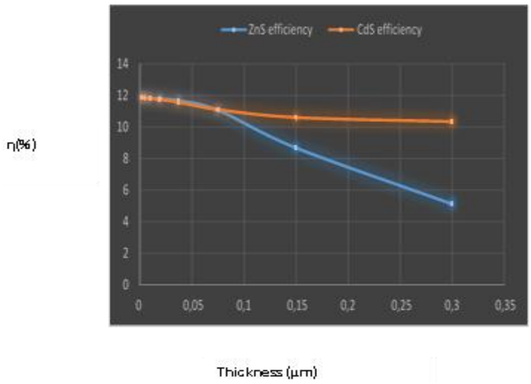

Fig. 8. The effect of temperature in the efficiency of Zinc Sulfied and Cadmium Sulfied buffer Buffer layer.

We can notice from this Graph that for small thickness (between 23 nm and 75 nm) of these materials, we can notice that the efficiency of CIGS-based solar cells, using ZnS as buffer layer, is relatively more much than the efficiency of solar cells using CdS as buffer layer, for smallest thickness.

4. Conclusion

The performance of CIGS-Based SOLAR cells, has been examinated. The highest power conversion efficiency is achieved 11.88% (Voc=0.5535v, Jsc=33.00085 mA/cm^2, FF=0.6503) for 1 µm thickness of absorber layer in the proposed material.

It can be seen that the buffer layer affects the efficiency and performance of photovoltaic solar cells, when it is subjected to changes in temperature and the thickness of said layer. We can notice that ZnS Buffer layer can be an alternatif material of CdS, and its application is more usefull than CdS buffer layer.

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