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RESEARCH ARTICLE

SIMULTANEOUS EFFECT OF SDL AND MOSE₂ LAYERS ON CIGS SOLAR CELL PERFORMANCE AND STRATEGY FOR IMPROVING ULTRA-THIN CIGS SOLAR CELL PERFORMANCE

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Abstract

In this paper, based on numerical simulation, the SCAPS-1D software was used to simultaneously study the influence of the surface defect layer (SDL) and the molybdenum diselenide layer (MoSe₂) on the performance of the CIGS solar cell. These two defects layers are respectively formed at the front interface (CdS/CIGS) and the back interface (CIGS/ Mo) by atomic inter-diffusion. Simultaneous analysis of SDL and MoSe₂ layers thickness revealed that optimum performance is achieved for 10 nm thickness of SDL layer and 35 nm thickness of MoSe₂. A study of the gap energy revealed that optimum performance is obtained for 1.25 eV energy gap SDL layer and 1.35 eV energy gap of MoSe₂ layer. Next, a performance study of the ultra-thin CIGS solar cell with optimized SDL and MoSe₂ layers was carried out. It was found that the presence of the SDL and MoSe₂ layers optimized improves the electrical performance of the ultra-thin CIGS solar cell.

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INTRODUCTION:-

In CIGS-based thin-film solar cells, the front interface CdS/CIGS plays an important role in the separation of electron-hole pairs, and the back interface CIGS/Mo is a zone of very high recombination, particularly for ultra-thin solar cells. Defects at these interfaces can make a significant contribution to improving the performance of CIGS-based thin-film solar cells. At the front interface CdS/CIGS and back interface CIGS/Mo, atomic inter-diffusion is observed[16]. At the front interface CdS/CIGS, cadmium (Cd) diffuses into the CIGS absorber and selenium (Se) diffuses into the CdS buffer layer [5]. In addition to the diffusion of cadmium (Cd) into the absorber, cadmium (Cd) diffuses into the surface regions of the CIGS absorber. Wada et al. showed the contact between Mo and CIGS to be ohmic, owing to the formation of an intermediate MoSe₂ layer during CIGS deposition [33]. At the back interface CIGS/Mo, selenium (Se) from the absorber diffuses to the surface regions of the back contact (molybdenum) due to its permeability[17, 34]. This phenomenon occurs during the CIGS deposition process on the molybdenum back contact [35]. Several X-ray photoelectron spectrometry (XPS) studies have shown the presence of very thin indium-rich (CuIn₃Se₅) n-type layers on the surface of the CIGS absorber [4, 29]. This thin layer, identified as a surface defect layer (SDL), has a different composition to that of the CIGS absorber volume[11]. Many studies agree that the SDL contributes to better adhesion between the Mo and the glass substrate[14, 33]. The layer acts in a beneficial way by changing the Schottky-type CIGS/Mo hetero-contact into an ohmic-type contact[14, 27]. Three factors may be responsible for the formation of the MoSe₂ layer. This layer may be due to the pressure during molybdenum sputtering [17, 18], to the concentration of sodium present in the soda-lime glass that diffuses into the CIGS

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absorber[33, 34], and finally to the selenization temperature [1]. Several studies have shown that the performance of ultra-thin CIGS-based solar cells is poor. However, what influence can the SDL and MoSe₂ layers have on CIGS solar cell performance? What influence might the thickness and band gap of these two layers have on CIGS solar cell performance? Can optimal values for the thickness and gap energy of these two defect layers improve the performance of the ultra-thin CIGS solar cell? In this paper, we will simultaneously investigate the influence of the thickness and gap energy of the SDL and MoSe₂ layers on CIGS solar cell performance. Subsequently, a strategy for optimizing the performance of the ultra-thin solar cell with optimized SDL and MoSe₂ layers will be made.

Material and Methods:-

Numerical simulation is a method used by researchers to study the impact of optoelectronic parameters on solar cell performance without actually performing an experiment. It makes it possible to characterize the behavior of a PV solar cell without performing an experiment. It reduces PV solar cell manufacturing costs. In this study, we plan to use the SCAPS-1D software [17]. to carry out our numerical simulations. The choice of this software lies in the fact that there is a good compromise between experimental results and numerical simulation[21, 23]. The SCAPS-1D software uses the finite-difference method with well-defined boundary conditions to solve the basic equations of the poisson equation, the electron continuity equation and the hole continuity equation[20]. The Poisson equation is a second-order partial differential equation (PDE) and is given by the following relation :

$$\nabla J_n = q[R(x) - G(x)] + q \frac{\partial n}{\partial t}$$

$$\nabla J_p = q[G(x) - R(x)] + q \frac{\partial p}{\partial t}$$

$\epsilon = \epsilon_0 \cdot \epsilon_r$ is the dielectric permittivity with ϵ_0 is the permittivity of the vacuum and ϵ_r is the relative permittivity of the material and ρ is the volume density of the free charges. $G(x)$ and $R(x)$ are respectively generation and recombination rates of electrons and holes, J_n and J_p are the densities of electron currents and holes.

n and p are the densities of electron and holes, \vec{E} is electrical field and V is electrical potential.

CIGS-based thin-film solar cells are heterojunction cells in which the p-type CIGS is the cell's absorber. The CIGS absorber is the most important layer of the device and occupies most of the volume of the solar cell [10, 26]. On this absorber, an n-type CdS buffer layer provides the P-N junction. A layer of high-resistivity transparent conductive oxide (TCO) is deposited on the buffer layer. As the TCO layer, we used a thin layer of intrinsic zinc oxide (i-ZnO) onto which we deposited a thick layer of aluminium-doped zinc oxide (ZnO:Al). The assembly is deposited on a substrate, which is the mechanical support. Generally speaking, soda-lime glass is the most widely used substrate in high-efficiency CIGS cells because of its properties compatible with the CIGS absorber[4, 28]. Ni/Al and Mo ohmic contacts are added to collect photo-generated electrons and holes. The structure of such a solar cell is shown in Figure 1 a.

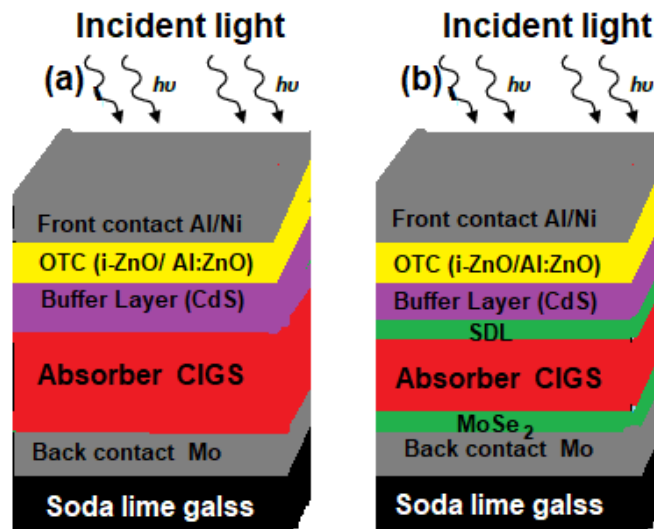


Figure 1:-Solar cell structure (a) without SDL and MoSe₂ layers and (b) with SDL and MoSe₂ layers used for numerical simulation.

At the front and back interfaces of the CIGS solar cell, the surface defect layer (SDL) due to atomic interdiffusion phenomena and the molybdenum diselenide layer due to diffusion of selenium from the absorber are shown in Figure 1.b. The equivalent band diagram of the solar cell with the SDL and molybdenum layers is shown in Figure 2.

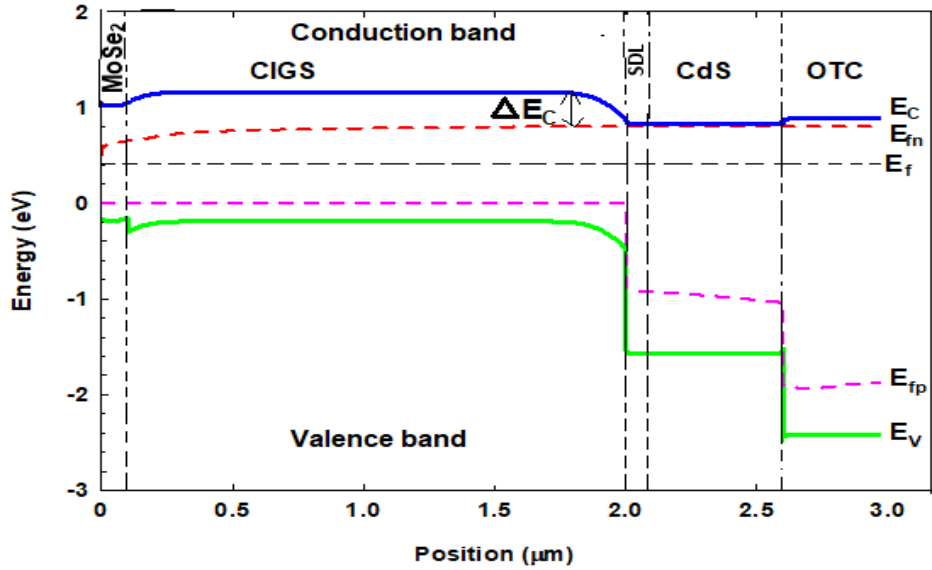


Figure 2:- Energy band diagram of solar cell with SDL and MoSe2 layers.

To characterize solar cell performance, we'll use the current-voltage (J-V) characteristic and quantum efficiency. The current-voltage (J-V) characteristic is used to analyze the electrical performance of solar cells. The curve of the solar cell's (J-V) characteristic is shown in Figure 3. Quantum efficiency (Q-E) describes the probability that an incident photon arriving at the surface of the device will create an electron-hole pair that can be collected and contribute to the device's current [7, 26].

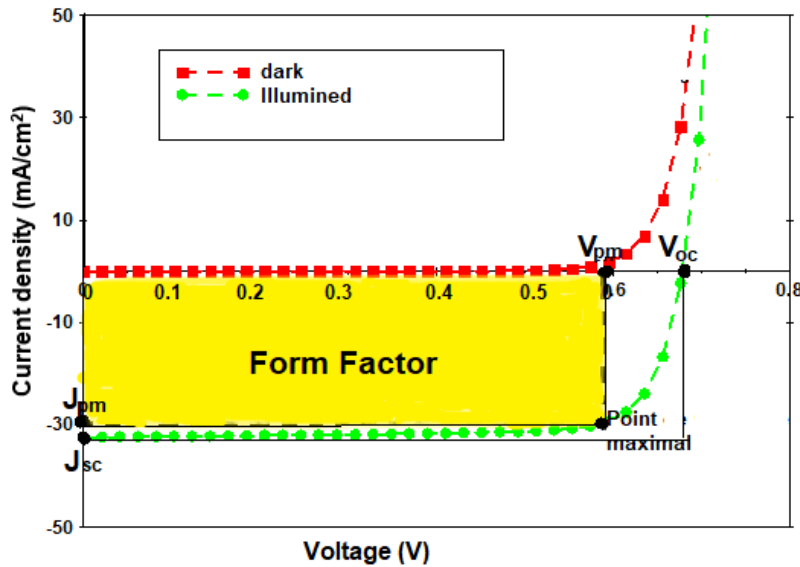


Figure 3:- Current-voltage (J-V) characteristic of a CIGS solar cell.

The properties of the various layers and interfaces used in the numerical simulation are summarized in Table 1.

Table 1:- The solar cells simulation parameters used in SCAPS-1D [22].

	ZnO/Al	CdS	CIGS
Thickness (nm)	100	50	2500

Band gap (eV)	3.3	2.4	1.25
Electron Affinity (eV)	4.55	4.5	4.5
Diélectric relative Permittivity	9.00	10	13.6
Effective densité of state in BC (cm ⁻³)	3.1 * 10 ¹⁸	3.1 * 10 ¹⁸	2 * 10 ¹⁸
Effective densité of state in BV (cm ⁻³)	1.8 * 10 ¹⁹	3.1 * 10 ¹⁸	1.5 * 10 ¹⁹
Electrons thermal velocity (cm/s)	2.4 * 10 ⁷	3.1 * 10 ⁷	3.9 * 10 ⁷
Holes thermal velocity (cm/s)	1.3 * 10 ⁷	1.6 * 10 ⁷	1.4 * 10 ⁷
Electrons Mobility (cm ² /Vs)	100	72	100
Holes Mobility (cm ² /Vs)	31	20	12.5
Doping density (cm ⁻³)	1 * 10 ¹⁷ (D)	5 * 10 ¹⁷ (D)	1 * 10 ¹⁶ (A)

The properties of the SDL and MoSe2 layer are summarized in Table 2.

Table 2:- The parameters of SDL and MoSe2 used in SCAPS-1D[7].

	SDL	MoSe ₂
Thickness (nm)	Variable	variable
Band gap (eV)	Variable	variable
Electron Affinity (eV)	4.5	4.372
Diélectric relative Permittivity	13.6	13.6
Effective densité of state in BC (cm ⁻³)	3.1 * 10 ¹⁸	2.2 * 10 ¹⁸
Effective densité of state in BV (cm ⁻³)	3.1 * 10 ¹⁸	1.8 * 10 ¹⁹
Electrons thermal velocity (cm/s)	3.1 * 10 ⁷	10 ⁷
Holes thermal velocity (cm/s)	1.6 * 10 ⁷	10 ⁷
Electrons Mobility (cm ² /Vs)	72	100
Holes Mobility (cm ² /Vs)	20	25
Doping concentration (cm ⁻³)	5 * 10 ¹⁷ (D)	10 ¹⁶

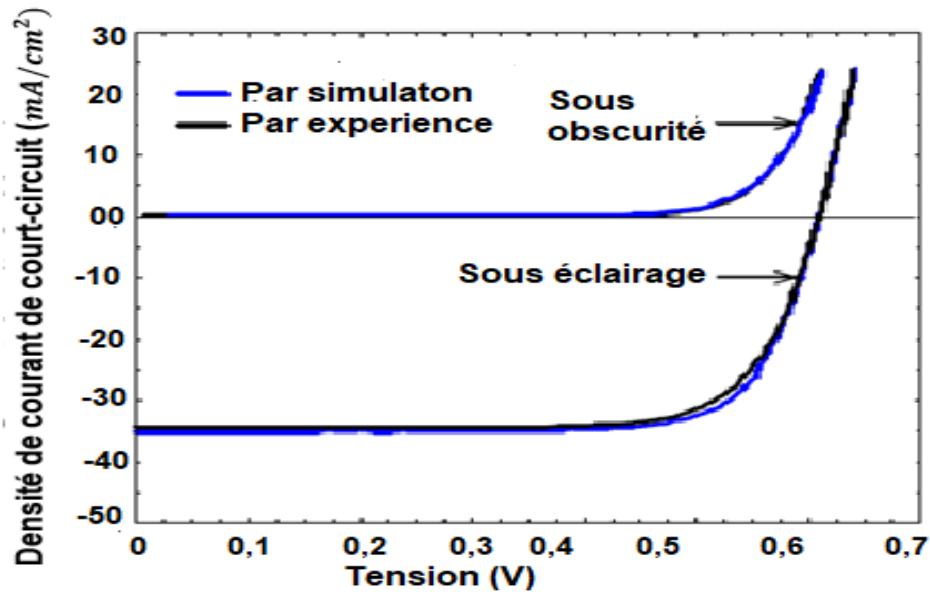


Figure 4:-J-V characteristic curves compared with experimental results from Pettersson and al. [21].

These properties were obtained from theoretical and experimental results [8, 22, 24]. The solar cell is illuminated under standard conditions by an AM 1.5G spectrum that accounts for direct and diffuse radiation and the solar cell temperature is maintained at 300K. To validate our results, we compared the J-V characteristic curves of our numerical simulation with those obtained experimentally by Pettersson. We can see that there is good agreement between these two results, as shown in Fig. 4, which leads us on to the results and discussion section.

Results and Discussion:-

Comparative study of CIGS solar cell performance with and without SDL and MoSe₂ layers.

In this section, we will study the performance of the CIGS-based thin-film solar cell with and without the presence of the surface defect layer (SDL) and the molybdenum diselenide (MoSe₂) layers. A good understanding of the physical parameters of the SDL layer and the MoSe₂ layer resulting from atom interdiffusion phenomena can be a major asset in optimizing solar cell performance. The SDL layer contributes to improved adhesion between the back contact (Mo) and the soda-lime glass substrate [2, 14]. The SDL layer causes wide bending of the strips and contributes to improved cell performance [22, 30]. However, can the simultaneous presence of these defect layers at the front and back interfaces contribute to improving the performance of the CIGS solar cell? To carry out this work, we analyzed the performance of the CIGS solar cell through the J-V characteristic. The characteristic curves (J-V) of the CIGS solar cell with and without the layers and SDL are shown in Figure 5. The differences between the both characteristic curves (J-V) are rather small. In reality, it would be very complicated to measure differences between these both curves.

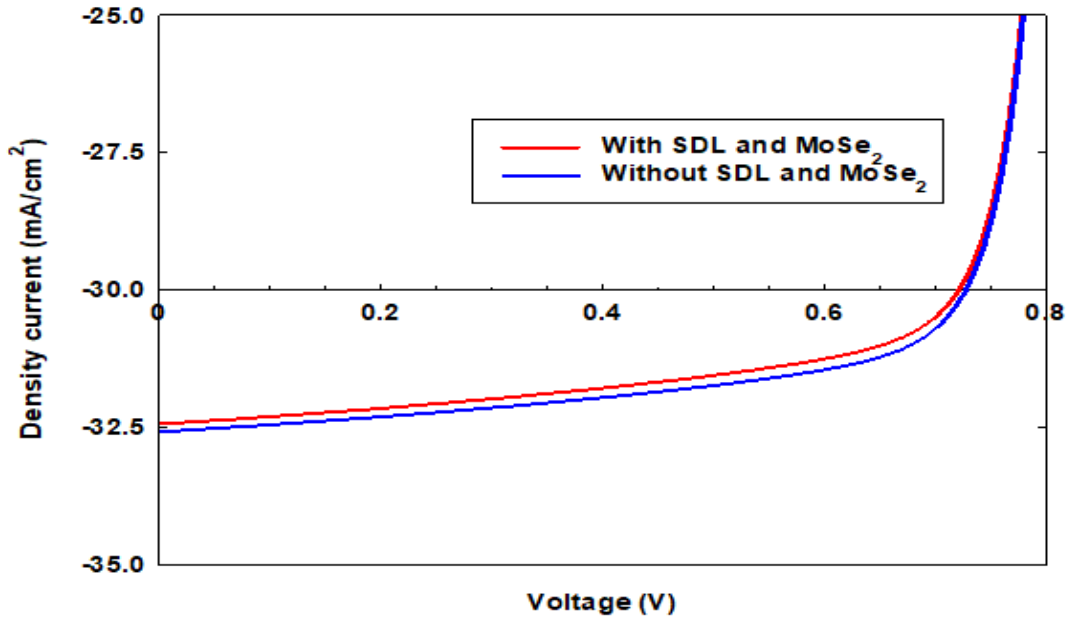


Figure 5:- J-V characteristics of solar cell performance with and without SDL and MoSe₂.

To solve this problem, we have extracted the electrical parameters of the solar cell with and without SDL layer and MoSe₂ from the J-V characteristic curve. These electrical parameters are summarized in Table 3.

Table 3:- Electrical parameters of the solar cell with and without the SDL and MoSe₂.

	V _{oc} (V)	J _{sc} (mA/cm ²)	FF (%)	η (%)
Without SDL and MoSe₂	1.1918	30.5585	59.50	21.67

With SDL and MoSe₂	1.1886	30.3412	59.54	21.47
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From this table 3, it's clear that the simultaneous presence of the SDL and MoSe₂ layers reduces the CIGS solar cell's performance. All the solar cell's electrical parameters are reduced. In the presence of the SDL and MoSe₂ layers, the solar cell's conversion efficiency falls from 21.6768% to 21.4020%, resulting in a loss in conversion efficiency $\Delta\eta = - 0.2\%$. The same applies to open-circuit voltage VOC and short-circuit current density JSC. This decrease in all electrical parameters can be explained by a reduction in the absorption of incident photons into electron-hole pairs in the presence of the SDL and MoSe₂ layers, as shown in figure 6.

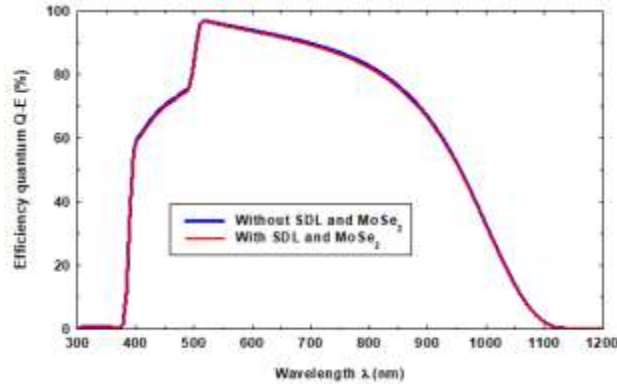


Figure 6:-Q-E quantum efficiency of solar cell performance with and without SDL and MoSe₂.

At the end of the study in this section, it appears that the presence of the SDL and MoSe₂ layers reduces slightly the solar cell's performance. However, what influence can the thickness of the SDL and MoSe₂ layers have on the performance of the CIGS solar cell?

Influence of SDL and MoSe₂ layer thickness on CIGS solar cell performance.

In this section, we will simultaneously study the influence of SDL and layer thickness on CIGS solar cell performance, as shown in Figure 7. The SDL layer has an estimated thickness of between 50 nm and 100 nm (Li et al., 2012). To achieve this, we vary the thickness of the SDL and MoSe layers from 5 nm to 100 nm.

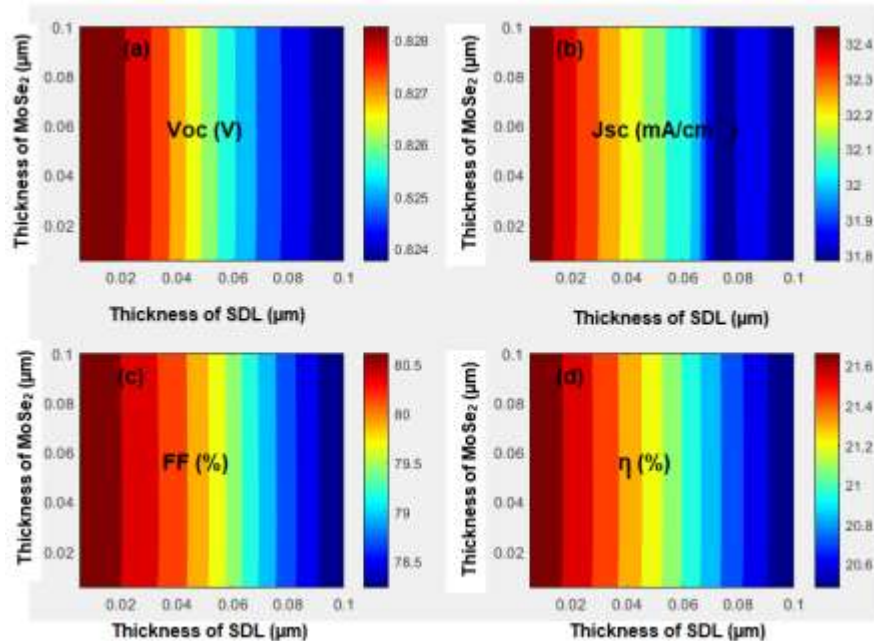


Figure 7:- Influence of thicknesses of SDL and MoSe₂ layers on electricals parameters.

In general, all the cell's electrical parameters follow the same progression, as shown in Figure 7. This study shows that solar cell performance decreases linearly with increasing SDL layer thickness. It also shows that solar cell performance varies very little with increasing layer thickness. From the following, we can affirm that the thickness of the SDL influences the performance of the CIGS solar cell more than the thickness of the layer. We can see that good performance is obtained for low values of SDL thickness ($W_{SDL} = 20$ nm). To obtain an optimum value for the layer thickness, we will vary its thickness from 5 to 100 nm, while fixing the SDL thickness at 15 nm.

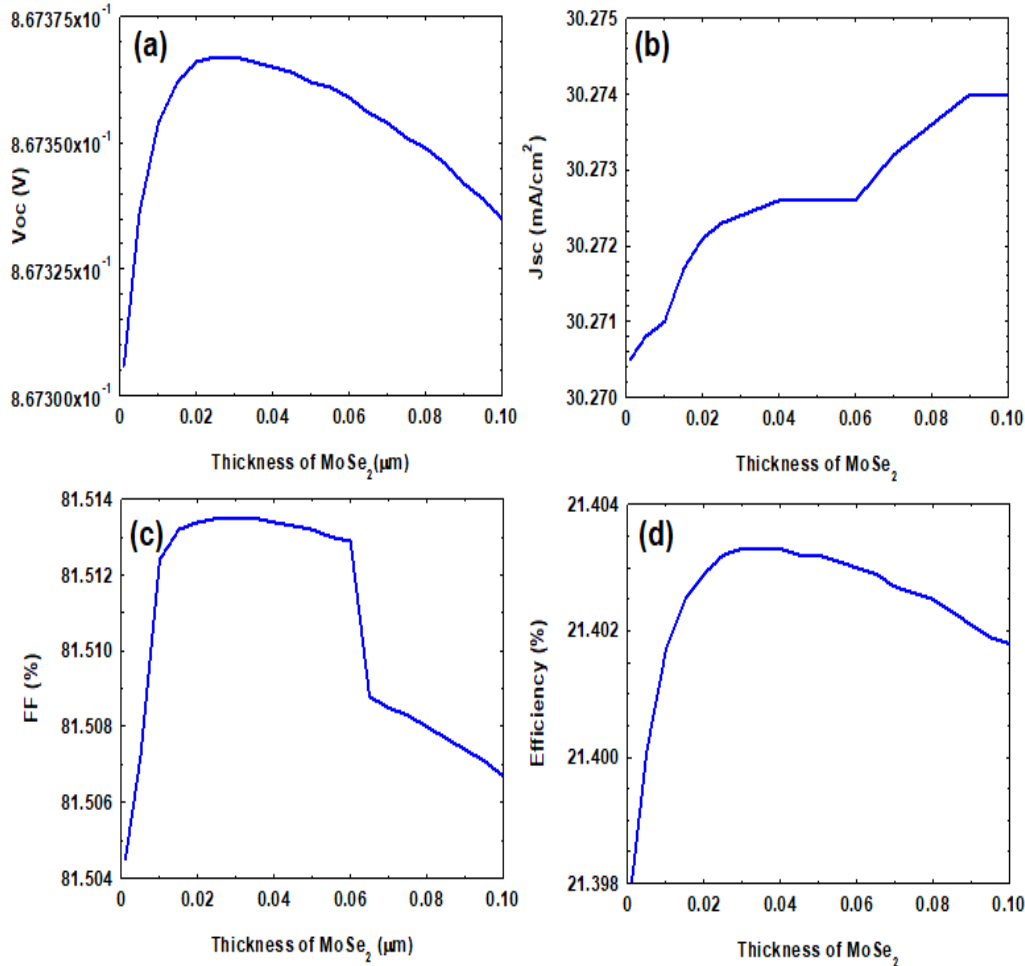


Figure 8:- Solar cell electrical parameters as a function of SDL layer thickness.

The electrical parameters of the solar cell vary only slightly as the layer thickness varies. For a layer thickness of less than 35 nm, all the solar cell's electrical parameters increase. Above 35 nm, the open-circuit voltage, efficiency conversion and form factor decrease. As for the density short-circuit current, it increases. Optimum performance of the CIGS cell is achieved at a layer thickness of between 30 and 40 nm. At the end of this study, it appears that optimum performance of the CIGS solar cell is obtained for low SDL and MoSe₂ layers thicknesses of the order of 15 nm and 35 nm respectively. However, what influence can the gap energy of the SDL and MoSe₂ layers have on CIGS solar cell performance?

Influence of gap energy of SDL and MoSe₂ layers on CIGS solar cell performance.

The numerical simulation carried out in this section will focus on the gap energy of the MoSe₂ and SDL layers, varying them from 1.0 eV to 1.45 eV and 1.0 eV to 1.5 eV respectively. Varying the gap energy of the MoSe₂ and SDL layers influences the J-V characteristic of the solar cell, as shown in Figure 9.

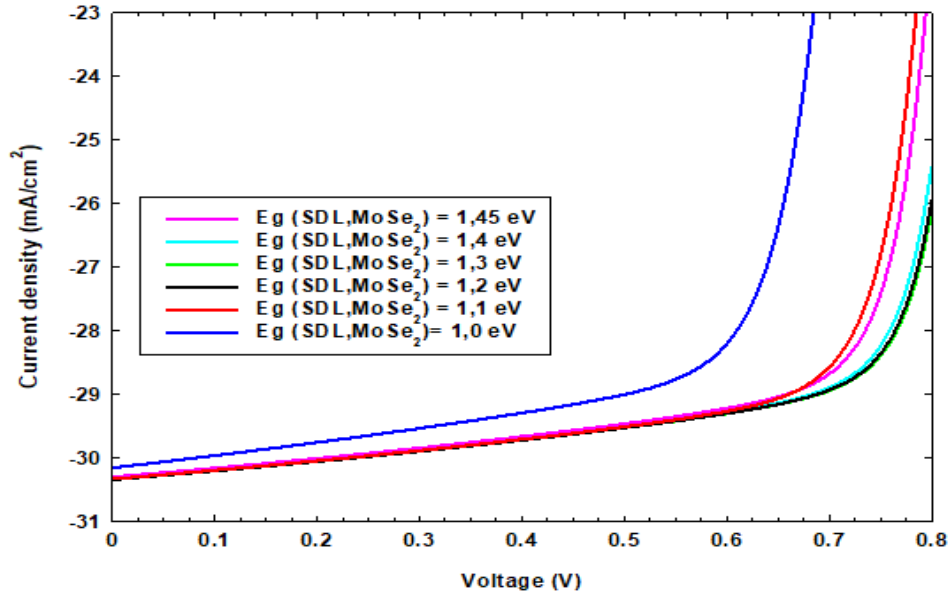


Figure 9:-J-V characteristic of solar cell for different energy bandgaps of SDL and MoSe₂ layers.

For a better understanding of the J-V characteristic curves, we have extracted the electrical parameters. These electrical parameters were then used to construct the curves shown in Figure 10. Figure 10.b shows that la density current short-circuit (Jsc) decreases when gap energy is less than 1,25 eV ($E_g(\text{SDL}) < 1,25\text{eV}$), whatever the gap energy of MoSe₂. Above this value, the Jsc is almost independent of the SDL and MoSe gap energy. Electrical parameters such as open-circuit voltage (Voc), form factor (FF) and solar cell efficiency (η) decrease when gap energy of SDL is less than 1,25 eV ($E_g(\text{SDL}) < 1,25\text{eV}$) and when gap energy of MoSe₂ is greater than 1,35 eV ($E_g(\text{MoSe}_2) > 1,35\text{eV}$).

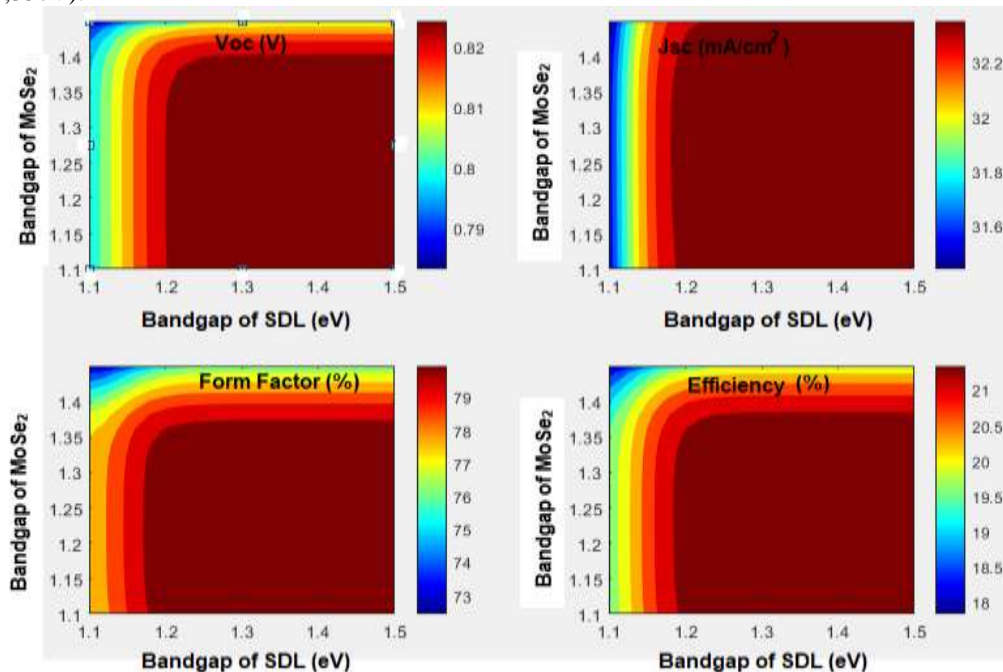


Figure 10:- Influence of gap energy of SDL and MoSe₂ layers on electrical parameters.

At the end of this study, it was found that optimum performance of the CIGS solar cell is obtained for $E_g(\text{SDL}) = 1,25\text{eV}$ and $E_g(\text{MoSe}_2) > 1,35\text{eV}$. These electrical parameters will be used to design a solar cell with optimized SDL and MoSe₂ layers.

Comparative study of the performances CIGS solar cell

The study carried out in the previous sections shows us that there is an improvement in the performance of the CIGS solar cell for optimum gap energies such as ($E_g(\text{SDL})=1,25\text{eV}$ et $E_g(\text{MoSe}_2)=1,35\text{eV}$) and for optimum thicknesses such as ($W(\text{SDL})=10\text{ nm}$ et $W(\text{MoSe}_2)=35\text{ nm}$). These optimum values were then used to develop a new solar cell with optimized SDL and MoSe₂ layers. In this section, we will compare the performance of the new solar cell with optimized SDL and MoSe₂ layers with that of the solar cell with SDL and MoSe₂. The simulation results are summarized in Table 4.

Table 4:- Electrical parameters of the solar cell with and without the SDL and MoSe₂ layers optimalis.

	$V_{oc}(V)$	$J_{sc}(mA/cm^2)$	FF(%)	$\eta(\%)$
With SDL and MoSe₂	1.1886	30.3412	59.54	21.47
With SDL and MoSe₂ optimalis	1.1216	30.4175	63.17	21.54

In this table, we can see that there is a clear improvement in the performance of the solar cell with the optimal SDL and MoSe₂ layers compared with the performance of the solar cell with the SDL and MoSe₂ layers. However, the performance of the solar cell with the SDL and optimal layers is lower than the performance of the solar cell without the SDL and MoSe₂ layers. However, can the use of the optimal SDL and MoSe₂ layers contribute to improving the performance of the ultra-thin CIGS solar cell?

Strategy for improving the performance of the ultra-thin CIGS solar cell.

To save on the raw materials indium and gallium, research is increasingly focusing on ultra-thin CIGS solar cells, i.e. with a relatively small absorber thickness ($W_{\text{CIGS}} < 0,5\ \mu\text{m}$). In order to improve solar cell performance, we should obtain a compromise between manufacturing cost and high-value efficiency. In this context, it is necessary to reduce the thickness of CIGS absorber [32]. Several studies have shown that CIGS solar cell performance decreases with decreasing absorber thickness [5]. It was clearly stated in Ref. [32] that growing an ultrathin layer of CIGS on Mo, with a thickness of less than $0.5\ \mu\text{m}$, can significantly degrade photovoltaic efficiency due to recombination losses and poor reflectivity at the CIGS/Mo interface. Several authors have proposed techniques to improve the performance of ultra-thin solar cells CIGS. Heriche et al. They have demonstrated that the inserted Si layer as the second absorber, boosts the solar cell efficiency from 16.39% to 21.3% [10]. For improve the performances of ultra-thin CIGS, Boubaker et al. has been also demonstrated that the addition silicon to reduce the thickness of CIGS improve the performances of ultra-thin CIGS with gallium content equal to 20 when the thickness of the absorber layer has been reduced to $0.75\ \mu\text{m}$ [10]. To carry out our numerical simulation, we set the absorber thickness of the ultra-thin CIGS solar cell at $0.5\ \mu\text{m}$. The electricals parameters of this numerical simulation are summarized in Table 5.

Table 5:- Electrical parameters of the ultra-thin solar cell with and without the SDL and MoSe₂ layers optimalis.

	$V_{oc}(V)$	$J_{sc}(mA/cm^2)$	FF(%)	$\eta(\%)$
Without SDL and MoSe₂	0.8935	24.8635	73.76	16.49
With SDL and MoSe₂ optimalis	0.9043	25.0575	73.57	16.63

From this table, we can see that the presence of the SDL and optimized MoSe₂ layers improves the conversion efficiency of the ultra-thin solar cell from 16.49% to 16.63%, i.e. a gain in conversion efficiency $\Delta\eta = 0.14\%$. The same applies to open-circuit voltage with a gain $\Delta V_{OC} = 0.01\text{ V}$ and short-circuit current density with a gain $\Delta J_{SC} = 0,19\%$. These performances can be explained by an increase in the absorption of incident photons with wavelengths between 500 nm and 900 nm, as shown in figure 8.

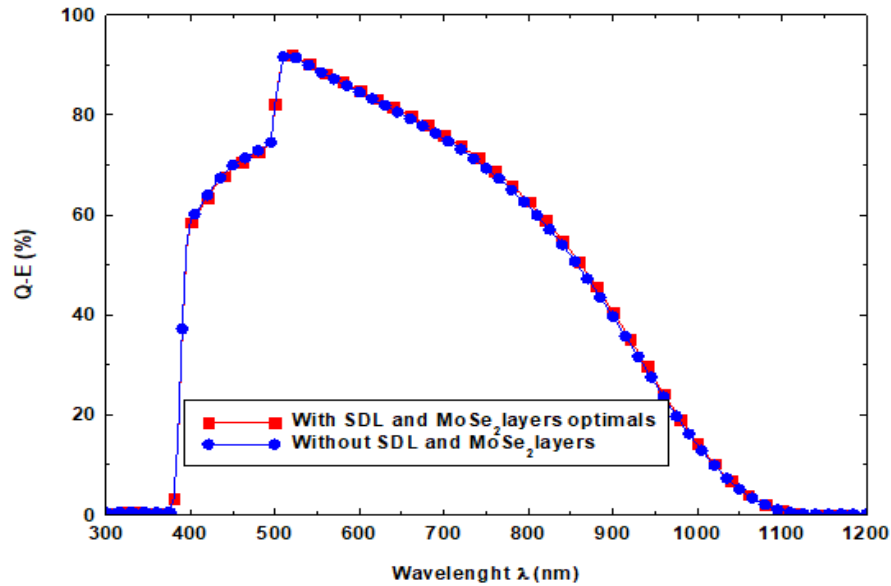


Figure 11:- Quantum efficiency of the performances of solar cell ultra-thin with the SDL and MoSe₂ layers and with the SDL and MoSe₂ layers optimals.

This increase in the electrical parameters of the solar cell ultra-thin with optimal SDL and MoSe₂ layers can be explained by the presence of the thin film that acts as an electron reflector at the back interface CIGS/Mo. This thin layer helps reduce charge carrier recombination at the back interface[28]. These performances may also be due to the presence of the thin SDL layer, which contributes to enlarging the space charge zone (SCZ). It may be explained by the reduced interaction between the holes collected at the back contact and the electrons photogenerated in the ultrathin absorber.

Conclusion:-

In our numerical simulation work, we have studied the performance of the CIGS-based thin-film solar cell with and without the presence of the SDL and MoSe₂ layers. This study shows that the performance of the CIGS solar cell improves for optimal gap energies such as (E_g (SDL)=1,25eV and E_g (MoSe₂)=1,35eV) and optimal thicknesses such as (W (SDL)=10 nm and W (MoSe₂)=35 nm). Next, a performance study of the ultra-thin solar cell with SDL and MoSe₂ optimized layers was carried out. This showed that the presence of the SDL and MoSe₂ layers optimized layers improved the conversion efficiency of the ultra-thin solar cell by 0.14%. The results obtained in this study provide a pathway to improve and design ultra-thin cells with high conversion efficiency.

Competing interests

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

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