Optimization of the Diameter of CdS Nanowires Embedded in a CZTS Buffer Layer under Different Solar Incidence Angles

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Abstract

Copper-zinc-tin-sulfide (CZTS) solar cells hold great promise in the production of solar energy.

A COMSOL Multiphysics simulation study of solar cells with cadmium sulfide (CdS) nanowires at different light angles is described in this study. The optimum diameter of CdS nanowires is 40 nm with a maximum absorption efficiency of 16.6%, a short circuit current density of 6.69 mA/cm^2, an open circuit voltage of 0.69 V, is obtained at an angle of incidence of light of 0°.

Keywords: CZTS; CdS Nanowires; Absorption; Efficiency; Short-circuit current density; Open circuit voltage.

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1. Introduction

Nanotechnology promises not only to increase efficiency but also to reduce the cost of solar cells (Tsakalakos 2008).

The incorporation of nanostructures in solar cells makes it possible to reduce the number of materials used in the absorbent layer, while improving absorption and therefore efficiency, thanks to strong light trapping and reduced reflection, at very low costs (Abouelmaaty M. Aly 2017). Indeed, the simulation on a thin-film silicon solar cell integrated with silver nanoparticles led to a yield of 16.18% (Afsaneh AsgariyanTabrizi et al. 2020).

Solar cells with p-n junction nanowires in a radial direction have high efficiency due to a large amount of trapped light (Kelzenberg et al. 2010). Add to this that by coupling incoming light into their localized resonances, nanowires can exhibit high absorption (Martin Foldyna et al. 2010). It has also been found that at short wavelengths, small-diameter nanowires are the most efficient at trapping light, while at long wavelengths, larger-diameter nanowires absorb light better (Martin Foldyna et al. 2013). This means that the choice of the diameter of the nanowires strongly influences the performance of the solar cell (Martin Foldyna et al. 2013). It is therefore necessary to find an optimal value of the diameter of the nanowires for all the wavelengths and under different angles of incidence of the light beams. Note also that regarding cell performance, vertical nanowire arrays have high tolerances to geometry changes compared to other cells (Martin Foldyna et al. 2013). This is very important for fabrications of nanowire solar cells which cannot guarantee the uniformity of the geometric dimensions of the nanowire arrays. Further still, Mohammadreza Khorasaninejad et al. have shown, for example, that at a light incidence angle of 70°, a nanowire length of 650 nm, and a nanowire pitch of 100 nm less than twice its diameter, nanowires with a diameter greater than 40 nm stand completely vertical, while nanowires with small diameters less than 15 nm bend conically (Mohammadreza Khorasaninejad et al. 2012). Indeed as the diameter of the nanowires increases, they undergo increased forces, called van der Waals forces whose energy dependence is given by equation (11), which must be compensated by an increased rigidity in the nanowires so that they can remain vertical (Mohammadreza Khorasaninejad et al. 2012 ; Volder et al. 2010 ; Israelachvili 2011 ; Lennart 1997).

$$W = \frac{AL\sqrt{d}}{24\sqrt{2}(P-d)^{3/2}} \quad (1)$$

Where A is the conventional Hamaker's constant, which has been taken as 8.03×10^{-20} J for silicon, l is the length, d is the diameter, and P is the pitch.

Note that the ratio W/A is unitless and depends only on the geometric parameters (L, d, p) of the model nanowires. The W/A ratio, therefore, has a lower limit and an upper limit depending on the values of the diameter d and can affect the performance of the cell. It is therefore appropriate to take an interest in it.

Note that for an efficient cell, the researchers were also interested in the ratio of the diameter to the pitch of the nanowires (Long Wen et al. 2011; Sambuddha Majumder et al. 2022). This is how Sambuddha Majumder et al. showed that by keeping the diameter (d) of the nanowires constant equal to 180 nm and by varying the pitch (p) of the nanowires, an increase in the ratio d/p from 0.4 to 0.6 led to an increase in l absorption from 80% to 90%, but also a decrease in efficacy from 27% to 13% (Sambuddha Majumder et al. 2022). This, therefore, requires finding an optimal d/p ratio. Thus, the closer the edges of the nanowires are, the better the absorption, and the worse the efficiency; it is, therefore, necessary to find an optimal distance from the edges of the nanowires. All these remarks have led to an interest, for each diameter d of the nanowires, in parameters such as d/h and p-d, the idea of which is very close to that of the geometric filling factor. Thus, in this study, we are interested in the only ratio that can include the three parameters p, d, and h at the same time.

However, the choice of the material of the nanowires and that of the absorbent layer also remains an important issue. CZTS-based solar cells are currently being investigated in several scientific studies as an absorbent material in thin-film solar cells (Hironori Katagiri et al. 2009) since CZTS is a semiconductor with a Kesterite-like structure and a good band gap of 1 .4 to 1.6 eV and a high absorption coefficient of more than 10^4 cm^{-1} with a refractive index of 2.72 (Wang et al. 2011 ; Nabeel A. Bakr 2016). In most solar cells, to facilitate the transition of electrons from the absorber to the window, a fairly thin buffer is used, generally between 50 and 200 nm thick, and which has a band gap between the absorber and the window so the conduction band is very small. The buffer also improves the interface between the absorber and the window, thereby reducing the recombination rate of holes and electrons (Eisele et al. 2003). It should be noted that the use of nanowires as a buffer layer further improves the efficiency of solar cells.

Cadmium sulfide (CdS), although it contains cadmium Cd (a toxic product), is a good choice to act as a buffer layer because it improves the interface with the absorber while ensuring strong transmission in the region of certain wavelengths. It also has a band gap of 2.4 eV and absorbs photons whose wavelength is less than 590 nm (Farhana Anwar 2017).

Recent research has shown that nanowires are able to concentrate solar energy with a much more efficient conversion rate than expected. Many scientific researchers, as in this study, are increasingly interested in CdS nanowires as a buffer layer (SOBONA 2014).

The experiments and studies carried out by Weiwei Sun on solar cells based on ZnO/CdS Core-Shell with the CZTS absorber made it possible to obtain an efficiency of 11% thanks to a 3D simulation (Weiwei Sun et al. 2013). On the other hand, using 1D simulation, those carried out by Dr. Hongmei Dang on the CdS-CdTe nanowire achieved an efficiency of 22.26% (Hongmei Dang 2015).

This study is focused on the optimization of the diameter and its relation with other geometrical parameters of the nanowires under different angles of incidence of the light and the determination of the electrical performances of the cell. It is based on the Comsol-Multiphysics simulation (COMSOL Multiphysics 2017 ; COMSOL Multiphysics 2018).

2. Materials and Methods

In this study, the following structure Mo \ CZTS \ CdS-nanowires \ ZnO \ Al: ZnO were considered. Here, zinc oxide (ZnO) constitutes the window layer. For good conductivity, the ZnO layer doped with aluminum (Al: ZnO) is used on the ZnO layer. The thin space between the molybdenum layer (Mo) and the CZTS layer which is molybdenum disulfide (MoS2) was also taken into account for the simulation.

In his work, CZTS thin films were prepared by sputtering Cu-Zn-Sn metal precursors from a single target, followed by sulfurization in sulfur vapor (COMSOL Multiphysics 2017).

The technique of manufacturing CdS nanowires is identical to that made by Dr. Hongmei Dang for his doctoral work (COMSOL Multiphysics 2018). The space between the nanowires is filled with CZTS.

Figure 1 shows the structural model of the studied solar cell, with CdS nanowires embedded in a CZTS buffer layer. CZTS is the p-type absorber layer. The Windows layer ZnO is n-type, and Al: ZnO is a transparent conducting oxide (TCO) layer.

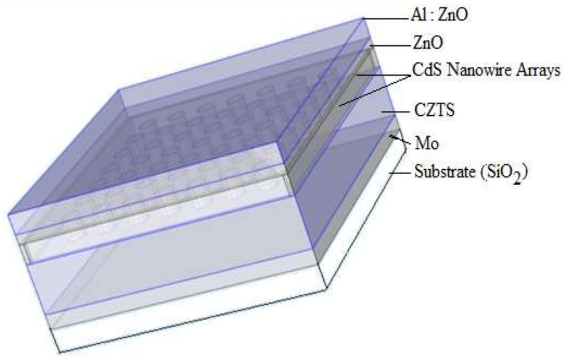

Figure 1. Device structure of CZTS- solar cell with CdS nanowires embedded in a CZTS buffer layer.

Solar panels generally do not operate exactly under an atmosphere thickness, if the sun is at an angle to the Earth's surface, the effective thickness will be greater. An Air Mass (AM) number representing the spectrum at mid-latitudes is therefore much more common. In this work, for solar radiation, we have considered the Solar Irradiance Spectra AM1.5 whose solar zenith angle is 48.2 ° (Oriel Jan 5, 2022).

By integrating solar spectral irradiance from 200nm to 2000nm using Comsol Multiphysics, we obtain a power density equal to $998.93\ \mathrm{W/m^2} \approx 1000\ \mathrm{W/m^2}$.

This study involves COMSOL Multiphysics, which uses the finite element method to solve the electromagnetic fields in the modeling fields. Assuming that the fields vary sinusoidally in time at a known angular frequency and that all the properties of the materials are linear with respect to the intensity of the field, Maxwell's equations governing in three dimensions reduce to the following relation (Tsakalakos 2008 ; Abouelmaaty M. Aly 2017 ; Afsaneh AsgariyanTabrizi et al. 2020 ; Nicolas Innocenti 2009):

$$\nabla \times \left(\frac{1}{\mu_r} \nabla \times E\right) - k_0^2 \left(\varepsilon_r - \frac{i\sigma}{\omega \varepsilon_0} E\right) = 0 \quad (2)$$

Where E is the electric field as a function of x, y, and z; $k_0^2 = \frac{\omega^2}{c_0^2}$; μ_r is the relative permeability; ε_r is the relative permittivity; $c_0 = \frac{1}{\sqrt{\varepsilon_0 \mu_0}}$ is the velocity of an electromagnetic wave in a vacuum; $\varepsilon_0 = 8.85 \times 10^{-12}$ F/m is the permittivity in vacuum and σ is the electrical conductivity. For non-magnetic materials $\mu_r = 1$. The permeability constant is $\mu_0 = 4\pi \times 10^{-7}$ H/m.

E is a vector with components Ex, Ey, and Ez.

The relative index in the environment can also be defined by:

$$\breve{n} = n + ik \quad (2)$$

$$\breve{n} = \frac{c_0}{c} \quad (3)$$

Where c is the speed of light in the material and n and k are respectively the real part and the imaginary part of the refractive index $\breve{n}$.

The absorption A(λ) can be obtained from the solutions of the electric field E (λ) describing Maxwell's equation (Van Dam D et al. 2016):

$$A(\lambda) = \frac{1}{2} \int \frac{2\pi \varepsilon_0 c}{\lambda} |E(\lambda)|^2 \, \mathrm{Im}(n^2(\lambda)) dv \quad (4)$$

Where $\varepsilon_0 = 8.85 \times 10^{-12}\ \mathrm{F \cdot m^{-1}}$ is the vacuum permittivity, c= 299792458 m/s is the speed of light in vacuum, λ is the photon wavelength, and n is the complex refractive index. T(λ) being the incident light fraction transmitted on the substrate; by energy conservation, the reflection R(λ) is obtained through the following relation: From energy conservation, the reflection is calculated through the relationship (Haomin Guo et al. 2011):

$$R(\lambda) = 1 - T(\lambda) - A(\lambda) \quad (5)$$

To evaluate the absorption in the CdS nanowires, we calculated for each angle of incidence, the ultimate absorption efficiency η, as defined by Shockley and Queisser (Shockley et al. 1961):

$$\eta = \frac{\int_{\lambda_l}^{\lambda_g} I(\lambda)A(\lambda)\frac{\lambda}{\lambda_g}d\lambda}{\int_{\lambda_f}^{\lambda_u} I(\lambda)d\lambda} \quad (6)$$

Where I (λ) is the solar spectral irradiance of standard air mass 1.5 (AM1.5); λ_l = 200 nm is the negligible solar irradiance, λ_u = 2000 nm is the upper limit of the available data for the solar spectrum, λ_g = 516 nm is the edge of the CdS band and given by :

$$\lambda_g = \frac{hc}{E_g} = \frac{1240}{E_g} \quad (7)$$

λg is expressed in nm; Eg = 2.4 eV is bang gap of CdS

Where h = 6.626×10^{-34} Joules x sec = 4, $14125\text{x}10^{-15}$ eVs is the Planks Constant, and c=299792458 m/s is the speed of light in vacuum.

The effective refractive index was introduced for the model with CdS nanowires (Haomin Guo et al. 2011):

$$n_{eff} = n_{air}(1-f) + (n_{CdS})f \quad (8)$$

Where n_{air} is the refractive index of air, n_{CdS} is the refractive index of CdS,

$$FF = \frac{\pi d^2}{4P^2} \quad (9)$$

FF is the geometric fill factor, where d is the diameter of the nanowire, and P is the pitch of the nanowires. For our simulation P= 362.5 nm.

The defined current density J of solar cells can be given through the equation below (Breitenstein 2013):

$$J = J_0[\exp(\frac{eV}{KT}) - 1] - J_{sc} \quad (10)$$

Where J_0 is the saturation current density, V is the applied bias voltage, $\frac{KT}{e}$ is the thermal voltage equal to 25.69 mV at 25°C, and J_{SC} is the short current density under illumination.

The open circuit voltage (Voc) can be extracted from equation (10), by canceling the current density J.

The short-circuit current density, J_{sc} is calculated by integrating the photogenerated charges under solar irradiance, and given by (BaominWang et al. 2014 ; Honghui Shen 2012):

$$J_{sc} = \frac{e}{hc}\int_{\lambda_l}^{\lambda_g} \lambda A(\lambda)I(\lambda)d\lambda \quad (11)$$

Where e is the elementary charge, equal to $1.6\text{x}10^{-19}$ C (Honghui Shen 2012).

We use the structure Mo \ CZTS \ CdS Nanowires \ ZnO \ Al: ZnO, with respective thicknesses of 150 nm, 500 nm, 150 nm, 100 nm, and 200 nm. The following values 0 °, 15 °, 30 °, 45 °, 60 °, and 80 ° were chosen to vary the angle of incidence. The studies focused on the following nanowire diameters: 20 nm; 40 nm; 60 nm; 80 nm; 100 nm and 150 nm. The pitch and height (length) of the nanowires are 362.5 nm and 150 nm, respectively. The distance between the edges of neighboring nanowires varies according to their diameter. The model is based on a square base of dimension 3000 nm x 3000 nm.

We, therefore, used 49 nanowires of 150 nanometers in length each, which are evenly distributed on a flat surface of $9x10^6$ nm^2. We varied the diameter of the nanowire from 20 nm to 150 nm and the light incidence angle from 0° to 80°.

The refractive index (real part n and imaginary part k) of CZTS was extracted from the experience of Nabeel A. Bakr et al. (Farhana Anwar 2017) and processed by the WebPlotDigitizer simulator (WebPlotDigitizer 2015). Given that the performance of a nanowire solar cell depends in part on the geometric parameters of the nanowires, and therefore on the ability of the nanowires to remain vertical under the influence of van der Waals forces, characterized by a W/A coefficient, independent of the nature of the material and the angle of incidence of the sunlight, but dependent on the geometric parameters. This ratio increases with increasing diameter d and has limits. In order to know the optimal value of this W/A ratio, we calculated it according to the values of the diameter d of the nanowires by referring to equation (1).

Comsol Multiphysics, despite its slowness in simulation calculations, offers the possibility of modeling with different dimensions (1D, 2D, 3D) (Tsakalakos 2008 ; Abouelmaaty M. Aly 2017 ; Afsaneh AsgariyanTabrizi et al. 2020), of coupling with other physics, such as optics, thermal physics, etc. Comsol also allows direct access to certain terms of the equations. This greatly motivated the choice of this simulation software for this study.

3. Results and Discussion

We used an air layer with a height of 120 nm, to take into account the parameters of the air in the simulation. To observe the behavior of the electric field inside the model we chose the Alice representation of Comsol-Multiphysics. For the model with CdS nanowires, we only gave the results with the nanowire diameter of 100 nm because of the good results on this model.

Figure 2 shows the simulation result of the Comsol electric field in 3d Multislice in the model with an incidence angle of 0° and a CdS nanowire diameter of 100 nm. In this Figure 2, the electric field averages $1.3x10^3$ V/m on the surface of Al: ZnO; around $0.9x10^3$ in the CdS nanowire arrays layer, and the vicinity of the CZTS absorbing layer. It is important to emphasize that the field is uniform in the absorber. This means that the absorption in the absorber and the vicinity of the layer of CdS nanowire arrays are practically the same.

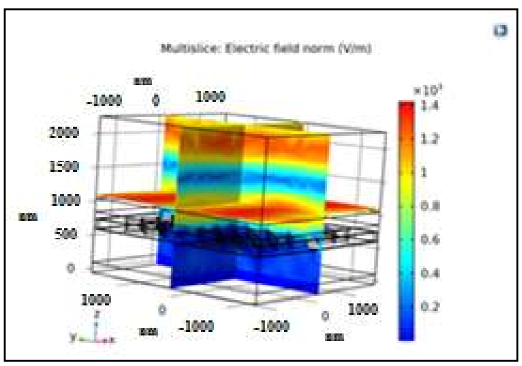

Figure 2. Electric field with an angle of incidences of 0° and a CdS nanowire diameter of 100 nm.

Figure 3 shows the result of the Comsol simulation Electric field in 3d Multislice in the model with an angle of incidence of 15 ° and a CdS nanowire diameter of 100 nm. In Figure 3, the electric field on the Al: ZnO layer is on average 30 V / m. In the CdS nanowire arrays and near the absorber, it is 25 V / m.

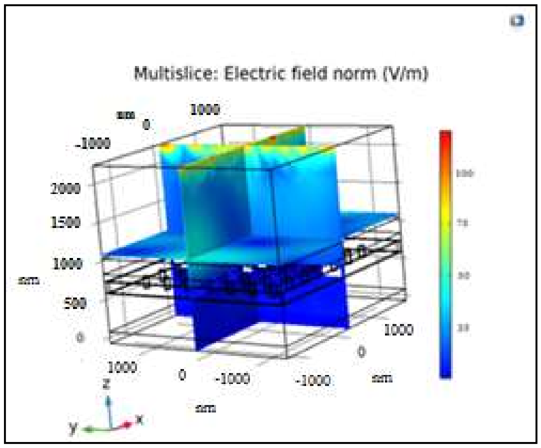

Figure 3. Electric field with an angle of incidences of 15° and a CdS nanowire diameter of 100 nm.

Figure 4 shows the result of the Comsol simulation Electric field in 3d Multislice in the model with an angle of incidence of 80 ° a CdS nanowire diameter of 100 nm. In this Figure 4, the electric field on the upper face of the layer Al: ZnO is equal to 20 V / m. It is equal to 8 V / m in the CdS nanowire arrays and near the absorber.

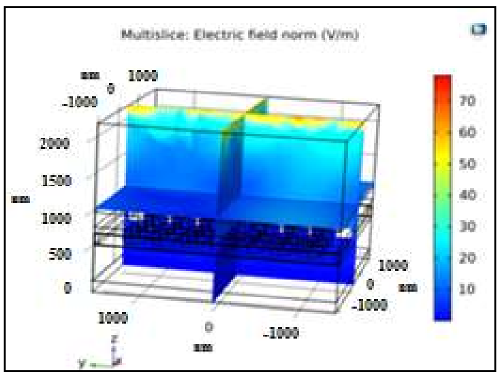

Figure 4. Electric field with an angle of incidences of 80° a CdS nanowire diameter of 100 nm

Note that the value of the electric field decreases when the angle of inclination increases. It is maximum at 0° at the upper surface of the model. The visualization of the results shows a symmetric behavior of the electric field in the nanowires.

According to equation (1), the absorption increases with the increasing integration of the edge of the electric field. This perfectly mirrors the graph of absorption versus wavelength. The figures below show absorption as a function of wavelength. These results were chosen among many others resulting from the simulation. L, d, and P being respectively the length (height), the diameter, and the pitch of the CdS nanowires (Figure 5), the W/A ratio equation (12)) is calculated according to the values of the diameter of the nanowires from the equation (1).

$$\frac{W}{A} = \frac{L\sqrt{d}}{24\sqrt{2}(P-d)^{3/2}} \tag{12}$$

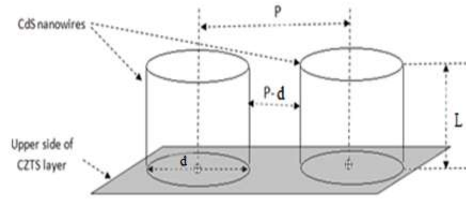

Figure 5. CdS nanowires on the upper side of the CZTS layer.

Table 1 shows the geometric fill factor and the W/A ratio as a function of the diameters of the nanowire.

Table 1. Geometric fill factors and W/A ratio as a function of nanowire diameters

d (nm)	**P** (nm)	**L** (nm)	**FF** (%)	W/A
20	362.5	150	0.24	0,0031
40	362.5	150	0.95	0,0048
60	362.5	150	2.15	0,0065
100	362.5	150	5.97	0,0083

Figure 6 shows the absorption with an angle of incidence θ = 0° (Figure 6(a)); 15° (Figure 6(b)); 45° (Figure 6(c)); (Figure 6(c)) 60° (Figure 6(d)) and 80° (Figure 6(e)) as a function of the wavelength from 200 nm to 2000 nm for different diameters d of the CdS nanowires. For θ = 0°, the light rays are perpendicular to the surface of the cell which is favorable to absorption. For the other angles of incidence of light, the light rays are inclined at the surface of the cell lowering the absorption. Therefore, the higher the angle of incidence, the better the absorption. On all the curves, the average absorption increases in the range of wavelengths between 200 nm and 380 nm (ultraviolet rays). As in nanowire solar cells in general, there is a slight increase in absorption from 800 nm and 1000 nm (in the infrared rays) (Steemit Elpatito Jan 5, 2022; The electromagnetic spectrum 2000; Wikipedia Dec 12, 2017). The best maximum absorptions are observed at 0°, the values of which are 97.20% at λ=390 nm and d=20 nm; 98.9% at λ=480 nm and d=40 nm; 97.92% at λ=380 nm and d=60 nm; 97.01% at λ=450 nm and d=100 nm.

Small-diameter nanowires (20 nm and 40 nm) trap more light at short wavelengths in the ultraviolet region (λ <400 nm) than large-diameter nanowires (60 nm, 80 nm), due to a very low geometric filling factor. In the infrared region (λ > 800 nm) the absorption for large diameters (60 nm and 80 nm) are on average the largest (Martin Foldyna et al. 2013). Indeed, the nanowires of small diameters (20 nm and 40 nm) have less reflection even if there is a small number of light trappings, we note an increase in the distance of travel of the photons, the energy being low in the long wavelength range, only a few photons reach the CZTS layer. This has the effect of weakening the absorption in this infrared zone.

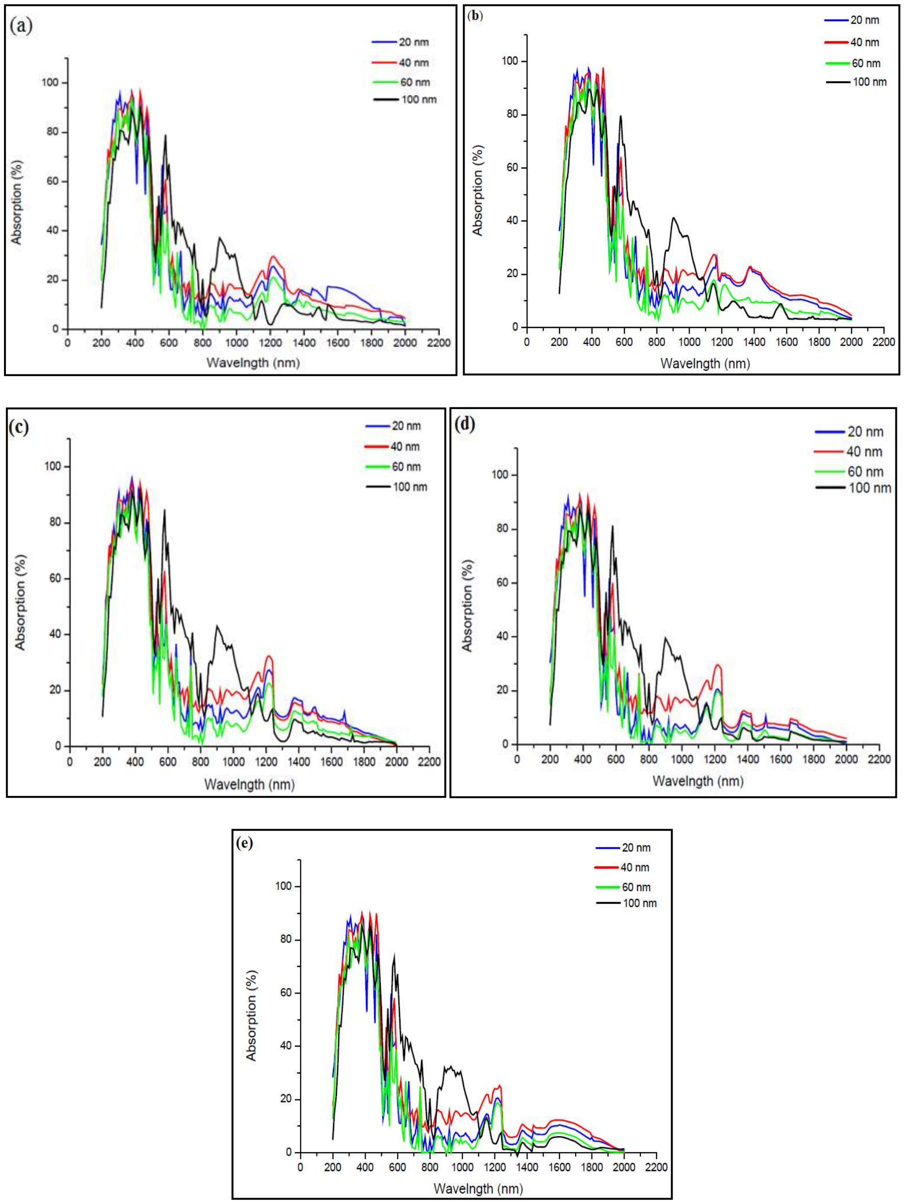

Figure 6. Absorption with an angle of incidence: (a) θ = 0°; (b) 15°; (c) 45°; (d) 60° and (e) 80° as a function of wavelength for different CdS diameters d.

Table 2 shows the summary of the maximum absorptions according to the diameters of the nanowires. It can be seen that the highest maximum absorption, which is 98.9%, was obtained by the nanowires with a diameter of 40 nm at a wavelength of 490 nm.

Table 2. Summary of the maximum absorptions according to the diameters of the nanowires

θ (°)	d = 20 nm		d = 40 nm		d = 60 nm		d = 100 nm	
	Maximum absorption (%)	**λ** (nm)	**Maximum absorption** (%)	**λ** (nm)	**Maximum absorption** (%)	**λ** (nm)	**Maximum absorption** (%)	**λ** (nm)
0	97,207	380	98,9	470	97,926	380	97,013	440
15	96,207	380	97,201	430	97,926	380	95,978	380
45	95,926	390	94,701	430	95,926	380	95,728	430
60	92,207	380	92,201	430	92,926	380	92,728	430
80	88,382	310	90,408	470	90,926	380	90,728	430

Figure 7 shows the ultimate efficiency curve for the different diameters of the nanowires as a function of the angles of incidence of the light. The more the angle of incidence increases, the more the ultimate efficiency decreases; due to the reduction of the surface visible to the sun's rays; therefore light rays on the surface of the cell. It is noted that 16.6% is the maximum yield value, which was obtained with the diameter of the nanowires of 40 nm at 0°. This can also be explained by the strong trapping of light in the nanowires of small diameters and reference to equation (6) by a high absorption in the nanowires with a diameter of 40 nm compared to the other diameters (Figure 6). At 15°, the ultimate efficiency of nanowires with a diameter of 20 nm almost equals that of nanowires with a diameter of 40 nm due to the weakening of solar radiation, and therefore of the number of photons participating in the radiation. At 100 nm in diameter, the distance between the nanowires is the smallest, which can affect light trapping and reflection rates. According to the simulation results (Figure 6) and equation (6), the efficiency obtained by nanowires with a diameter of 100 nm is the lowest. Note also that from a certain diameter value of the nanowires, a decrease or an increase in the diameter can lead to a decrease in efficiency in the nanowires (Martin Foldyna et al. 2013). This means that there is an optimal value of the diameters of the nanowires and an optimal distance between the edges of the nanowires, i.e. an optimal value of d, FF, and W/A. Analysis of the simulation results indicates that d = 40 nm, FF = 0.95% and W/A = 0.0048 are the best results of the efficient model.

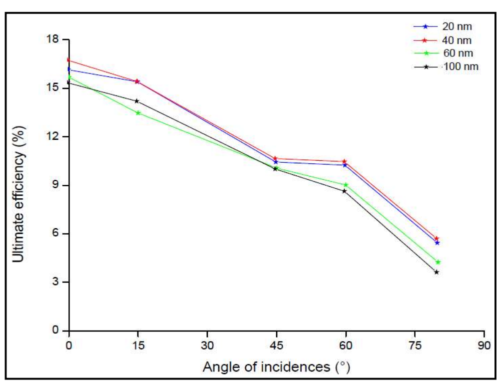

Figure 7. Ultimate efficiency as a function of angle of incidence.

Tables 3 and 4 respectively show the short-circuit current density (Jsc) and the open circuit voltage (Voc) obtained from the simulation and calculations (9) and (10).

Table 3. Short current density (mA/cm^2)

Angle of Inc.	Jsc d = 20 nm	Jsc d = 40 nm	Jsc d = 60 nm	Jsc d = 100 nm
0°	6.6238	6.6999	6.7109	6.8289
15°	5.2980	5.3891	5.4210	5.5215
45°	4.1824	4.2183	4.2239	4.2503
60°	4.4416	4.4136	4.2533	4.2269
80°	2.0239	2.1832	2.3518	2.3834

Table 4. Open circuit voltage Voc (V)

Angle of Inc.	Voc d = 20 nm	Voc d = 40 nm	Voc d = 60 nm	Voc d = 100 nm
0°	0.7042	0.6993	0.6098	0.5115
15°	0.6210	0.6027	0.4838	0.4682
45°	0.6072	0.6071	0.5462	0.4666
60°	0.6070	0.5883	0.5424	0.4312
80°	0.6478	0.6207	0.5419	0.4302

It is noted that the large diameters of nanowires have a high short-circuit current density due to a large coverage of incident photons therefore of the total surface of contact with the incident light. The smallest diameters have a high open circuit voltage due to a low electron-hole recombination rate and a low filling coefficient.

These results confirm the results of the experiments carried out by Mohammadreza Khorasaninejad et al. on solar cells with arrays of silicon nanowires which claim that when the diameter of the nanowires is not less than 40 nm, the nanowires are entirely ordered and vertical, and group together by deforming under the effect of van der forces Waals when diameter decreases; below 20 nm in diameter of the nanowires, the conical shape of the nanowires is visible; at 32 nm in diameter, even if the conical shapes of the nanowires are no longer achieved, gripping of the nanowires is still observed, which negatively affects the performance of the solar cell. Thus, through their experiments, Mohammadreza Khorasaninejad et al. also confirm that 40 nm is the optimal diameter for the vertical tenacity of the nanowires (Mohammadreza Khorasaninejad et al. 2012). These simulation results can be used for nanowire sizing in the fabrication of CZTS solar cells with CdS nanowire arrays integrated into a CZTS buffer layer.

3. Conclusions

In this work, we simulated the CZTS solar cell with CdS nanowire arrays integrated into a CZTS absorber by Comsol Multiphysics to identify and evaluate the parameters responsible for improving the efficiency of this cell. solar. We know that trapping light through nanowires increases the efficiency of solar cells. Since cell efficiency is related to uptake; it was, therefore, necessary to study absorption in the CZTS solar cell with an absorbing buffer structure of CdS nanowire arrays and a diameter/pitch ratio close to 0.4, therefore less than 0.5, as numerous studies suggest. The results of our simulations showed that the absorption, in general, increases in the ultraviolet region between 200 nm and 300 nm, often up to 420 nm, independent of the angle of inclination of the light and the diameter of the nanowires. . It generally decreases from wavelengths between 380 nm and 500 nm. The absorption curves also indicated that the best absorption is 98.9%, obtained at a wavelength of 490 nm for an angle of incidence of 0°, a diameter of CdS nanowires of 40 nm, a W/A ratio of 0.0048, and a geometric fill factor FF of 0.95%.

The short-circuit current density (Jsc) at 0° angle of incidence is 6.69 mA/cm2 for the diameter of the 40 nm nanowires, the highest value which is 6.82 mA/ cm2 is obtained with nanowires 100 nm in diameter. The open circuit voltage (Voc) at an angle of incidence of 0° is 0.60 V for the nanowires of 40 nm in diameter, the greatest value of 0.62 V being obtained with those of 20 nm in diameter.

In this work, the highest ultimate efficiency 16.6%, was obtained with the CdS nanowires with a diameter of 40 nm.

These results are very close to those obtained in the literature. The small difference observed is certainly due to poor adhesion and high series resistance in solar cells due to the MoS2 layer developed during sulfurization which can lead to an increase in the number of charge carrier recombinations near the contact. rear (COMSOL Multiphysics 2017). This problem, when studied in depth, can be solved by simulation.

It should also be noted that light trapping due to multiple ray reflections effectively increases the optical path length in the nanowires and improves the absorption efficiency. Moreover, the use of large values of the diameter of the nanowires penalizes the trapping of light and the small diameters of the nanowires are not very favorable to the absorption of light.

We can therefore conclude based on our simulation results that CZTS solar cells with CdS nanowire arrays embedded in a CZTS buffer layer must have a diameter/pitch ratio of less than 0.5 and a vertical tenacity ratio against the forces of van der Waals, W/A very close at 0.5%. These simulation results, although not yet experimentally tested, may be useful for nanowire sizing in the fabrication of these CZTS solar cells with CdS nanowire arrays integrated into a CZTS buffer layer.

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