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USING COMPUTER MODELS SCAPS-1D, THE INFLUENCE OF THE THICKNESS OF THE ABSORPTION LAYER ON THE PERFORMANCE OF A THIN-FILM SOLAR CELL (CCZTSE)

Wisam Yaseen Ali
Dept of Physics , College of Science ,University of Kirkuk ,Kirkuk,IQ.
wsamy905@gmil.com

Mohanad Q.Kareem
Dept of Physics , College of Science ,University of Kirkuk ,Kirkuk,IQ.
drmohanad33@uokirkuk.edu.iq

ABSTRACT

The solar cell (CCZTSe) was investigated using SCAPS-1D computer simulations, and it was discovered that the compound (CCZTSe) is one of the best compounds for photovoltaic absorption layers. Because of its adequate electrical and optical characteristics, the compound was shown to be more stable in the investigation. It was discovered that increasing the thickness of the absorption layer (CCZTSe) from (0.1-1 µm) raises the curve (I-V) and therefore increases the values of (V_{OC} , J_{SC} , FF , Ŋ) from (0.804766V, 33.73473553 mA/cm^2, 85.6023 %, 23.2398 %) to (0.816250V, 51.21920321 mA/cm^2, 85.8006 %, 35.87 %) Because the cell is perfect, it was discovered that the quantitative efficiency (QE) improves as the thickness of the absorption layer (CCZTSe) grows until it reaches (100 %) at a thickness of (1 µm).

Keywords: SCAPS-1D, CCZTSe, Back surface Layer (BSL), solar cell, conversion efficiency (Ŋ), Quantum efficiency (QE).

Introduction

One of today's primary issues is the scarcity of fossil fuels and hydrocarbons, as well as the negative effects of increased use on the environment, quality of life, and human health. As a result, it is critical to switch to other energy sources. One solution to this problem is renewable energy, and one of the most common kinds is solar. Solar energy is now widely available and exploitable because to photovoltaic (PV) technology [1]. The investigation of the suggested molecule (CCZTSe) in this research resulted in the development of novel solar cells, with a focus on thin-film cells to manufacture high-efficiency, low-cost cells. The compound is a Cu2ZnSnSe4 (CZTS) and Cu2CdSnSe4 (CCTS) alloy material with an energy gap of 1.05-1.5 eV [2]. And, according to the research, the energy gap of the compound (CCZTSe) containing (Cd) and (Zn) is within the range of (0.8-1 eV). As a result, the wavelength of spectral absorption in the infrared is extended. The goal of the study is to use computer modeling to develop a high-efficiency photovoltaic cell by varying the thickness of the absorption layer and its impact on the solar cell's performance. In 2021, Yuying Jiao et al. used a simulation approach to create an experimentally constructed solar cell (SCAPS-1D) employing (CCZTSe) as the absorption layer, (ZNO) as the window layer, and (CdS) as the buffer layer for an experimentally built photovoltaic cell (SCAPS-1D). The research revealed that the (CCZTSe) layer is a promising high-quality material for infrared ray response and detection[3].

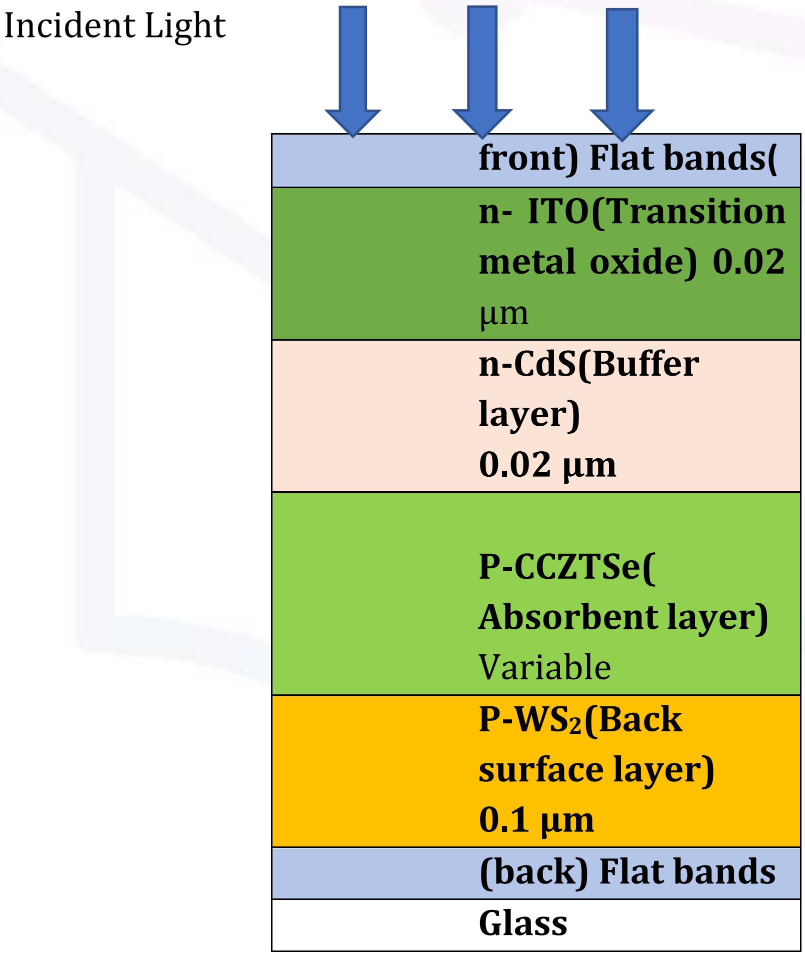

figure (1): Stages of study and design of the cell Solar

Simulation Process:

The computer is used to create a mathematical model that contains the model's basic parameters. Understanding novel semiconductors and structures, as well as projecting their quality and theoretical performance, may be made much easier through simulation modeling. As indicated in the picture, a simulation program (SCAPS-1D) was utilized to build a solar cell in this work .Over the years, computer modeling for solar devices has shown to be a beneficial method for researching and understanding photovoltaic device features such as optical, electrical, and mechanical aspects of complicated photovoltaic systems. By giving a collection of helpful information on how to adjust production settings to increase device performance, it also minimizes processing costs and researcher time spent on making solar devices. SCAPS-1D, a one-dimensional photovoltaic modeling program created in Electronics and Information Systems (ELIS) at the University of Ghent in Belgium and freely available to all photovoltaic researchers, is the subject of this study. A photovoltaic cell may be described as a collection of up to seven layers, each with its own set of attributes such as thickness, optical absorption, mobility, density, and fault distribution. A variety of common measures can be emulated, including I-V, QE, C-V, and C-f. For numerous forms of photovoltaic study, the program is freely accessible. The Poisson equation, the electron and hole continuum equation, and the SCAPS simulation are all predicated on solving these three semiconductor equations. The cell was investigated in its ideal condition (i.e., without flaws), because adding faults to the cell enhances or preserves electrical conductivity, yet imperfections frequently induce losses and diminish the cell's efficiency. The optical properties curve (QE) and the curve (I-V), which comprise the values (V_{OC} , J_{SC} , FF , η , QE), were derived by using the equations (1,2,3,4,5) [4] at room temperature (300 K).

$$\mathbf{V_{OC} = \frac{K_B T}{q} \ln\left(\frac{J_{Ph}}{J_0} + 1\right)}\text{----------------}\mathbf{(1)}$$

When there is no short circuit current, the (V_{OC}) is the maximum voltage obtained from the solar cells, implying that there is no contact via the photovoltaic cells according to the relationship. As a result, (V_{OC}) is a measure of recombination in photovoltaic cells[5].

$$\mathbf{J_{SC}(V) = J(V) + J_O \left(e^{qv/mk_BT} - 1\right)}\text{-----------}\mathbf{(2)}$$

When there is no load, the (J_{SC}) is the highest current flow in the solar cells. When the open circuit voltage (V_{OC}) is zero, (J_{SC}) has the highest value. The number of incoming photons, the optical spectrum, the accumulating potential, and the area of the photovoltaic cells all have a role[5].

$$\mathbf{FF} = \frac{J_{max} \cdot V_{max}}{J_{oc} \cdot V_{oc}} \text{------------------------}\mathbf{(3)}$$

Where the (FF) is the result of dividing the cell's maximum power (Jmax . Vmax) by the product of the resultant power from the product of (J_{SC} . Voc), and the acceptable value of (FF) for photovoltaic cells is between (70-85 %).

$$\eta = \frac{P_{max}}{P_{in}} = \frac{J_{sc} \cdot V_{oc} \cdot FF}{P_{in}} \quad \text{-----------------}\mathbf{(4)}$$

where (Ŋ) is used It may be defined as the product of dividing the photovoltaic cells' output power by the input power (the product of solar radiation intensity with the cell area).

$$\mathbf{QE} = \frac{R\lambda hc}{q\lambda}$$

hc/q=1.24 where is a constant value

$\mathbf{QE = 1.24} \left(\frac{R\lambda}{\lambda}\right)$ **---------- (5)** can be written:

Rλ: Response in units (A/W), λ: wavelength (nm)

Where the (QE) is the proportion of carriers generated in a photovoltaic cell to photons falling on the cell surface per unit wavelength falling on the cell surface, and it may be represented in wavelength and spectral response[6]. The photovoltaic conversion efficiency is now measured using a 1000 W/m^2 1.5AM spectrum, which has become a worldwide standard[4]. The input parameters utilized in the simulation software, which were adopted, are listed in table (1). The following are the findings of the published research: ITO (window layer): - It's the layer with a big energy gap and a high refractive index, which prevents light from refraction. To allow the most number of light rays to enter the cell, it is an n-type semiconductor compound[7]. BSL(WS_2): - Tungsten disulfide, also known as dichalcogen as a transitional element[8], is a non-toxic substance. It is the layer that aids in the return of electrons [9]. Cadmium sulfide (CdS) is a kind of cadmium sulfide. It is frequently employed as an insulating layer in solar cells to produce p-n junctions. It merged with the absorbent layer, resulting in extremely efficient cells[10].

Prameter	**symbol (unit)**	CCZTSe -P [11]	WS_2 -P [12]	CdS -n [13]	ITO-n [14]
Thickness	m) (μd	Variable	0.1	0.02	0.02
Band gap	Eg (eV)	0.9	1.29	2.4	3.6
Electron affinity	χ (eV)	4.4	4.05	4.2	4.1
Dielectric permittivity	$r\epsilon/\epsilon$	10	13.6	10	10
CB effective density of states	$N_C(cm^{-3})$	2.2 E+18	2.2 E+18	2.2 E+18	2 E+18
VB effective density of states	$N_V(cm^{-3})$	1.8 E+19	1.8 E+19	1.8 E+19	1.8 E+19
Electron thermal velocity	$V_n(cm/s)$	1.0 E+7	1.0 E+7	1.0 E+7	1.0 E+7
Hole thermal velocity	$V_P(cm/s)$	1.0 E+7	1.0 E+7	1.0 E+7	1.0 E+7
Electron mobility	$\mu_n(cm^2/v.s)$	60	100	100	50
Hole mobility	$\mu_p(cm^2/v.s)$	20	100	25	75
Shallow uniform donor density	ND (1/cm3)	0	0	1E18	1E18
Shallow uniform acceptor density	NA (1/cm3)	1E17	1E17	0	0

Table (1) :Parameters used for solar cell simulation: WS_2+ CCZTSe+CdS+ITO

Thickens μm	**V_{OC} V**	**J_{SC} mA/cm²**	**FF %**	**%η**
0.1	0.804766	*33.73473553*	85.6023	23.2398
0.2	0.810582	*41.88921132*	85.7630	29.1205
0.3	0.813124	45.89790077	85.7886	32.0169
0.4	0.814417	48.04326405	85.7971	33.5700
0.5	0.815140	49.27647288	85.8000	34.4635
0.6	0.815575	50.02990920	85.8011	35.0095
0.7	0.815851	50.51349179	85.8007	35.3597
0.8	0.816035	50.83761026	85.8006	35.5946

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0.9	0.816160	51.05859291	85.8009	35.7549
1	0.816250	51.21920321	85.8006	35.8712

Table(2) Cell properties when changing the thickness of the absorbent layer WS_2+ CCZTSe+CdS+ITO

Results and discussion:

The cell (WS_2+ CCZTSe+CdS+ITO) was examined and found to be defect-free. The absorbent layer (P-CCZTSe) thickness was modified from (0.1-1 μm). The layer BSL(WS_2) had a fixed thickness of (0.1 μm), whereas the layer (CdS,ITO) had a thickness of (0.02 μm), as shown in figure (2). (I-V). The (I-V) isotropic curve grows as the thickness of the absorbent layer increases. Higher layer thickness leads to increased absorption Photons with less energy than the blocked gap, and increasing the thickness leads to increased absorption Photons with less energy than the blocked gap[15].

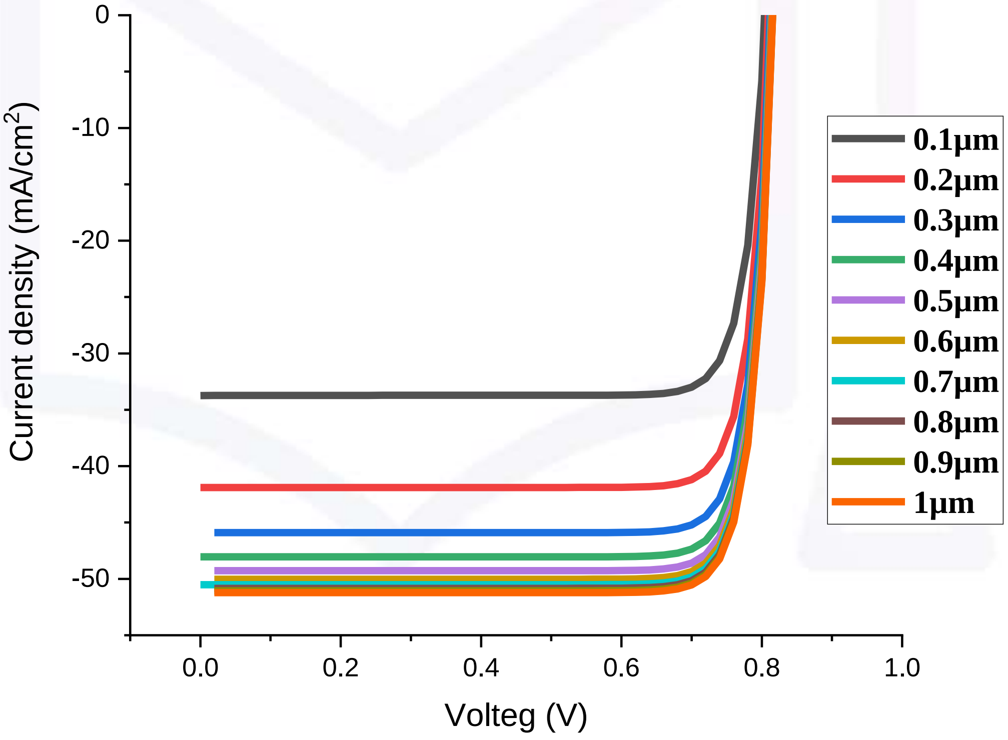

figure (2):The effectof the thickness of the P-CCZTSe absorbent layer on the properties (I-V)of the cell WS_2+CCZTSe+CdS+ITO

As for the quantum efficiency (QE), we see an increase in the quantum efficiency from (95.6 %) at thickness (0.1 µm) to (100 %) at thickness (1 µm) and wavelength at (300nm) as shown in figure (3), and one of the advantages of this type of cell is that the quantum efficiency (QE) does not depend on the distance of the barrier (p-n) from the surface, as the semiconductor material with a l is a semiconductor material with a Long-wavelength photons are profoundly absorbed in the absorption layer (P-CCZTSe), resulting in a high quantum efficiency of the produced electrons that is dependent on propagation length, as evidenced by an increase in the open circuit voltage and current density [16]. When the quantum efficiency drops at long wavelengths, it's because of absorption generated by the back reflection layer (WS_2), which helps to reduce the creation of pairs (electron-hall), lowering the quantum efficiency (QE).

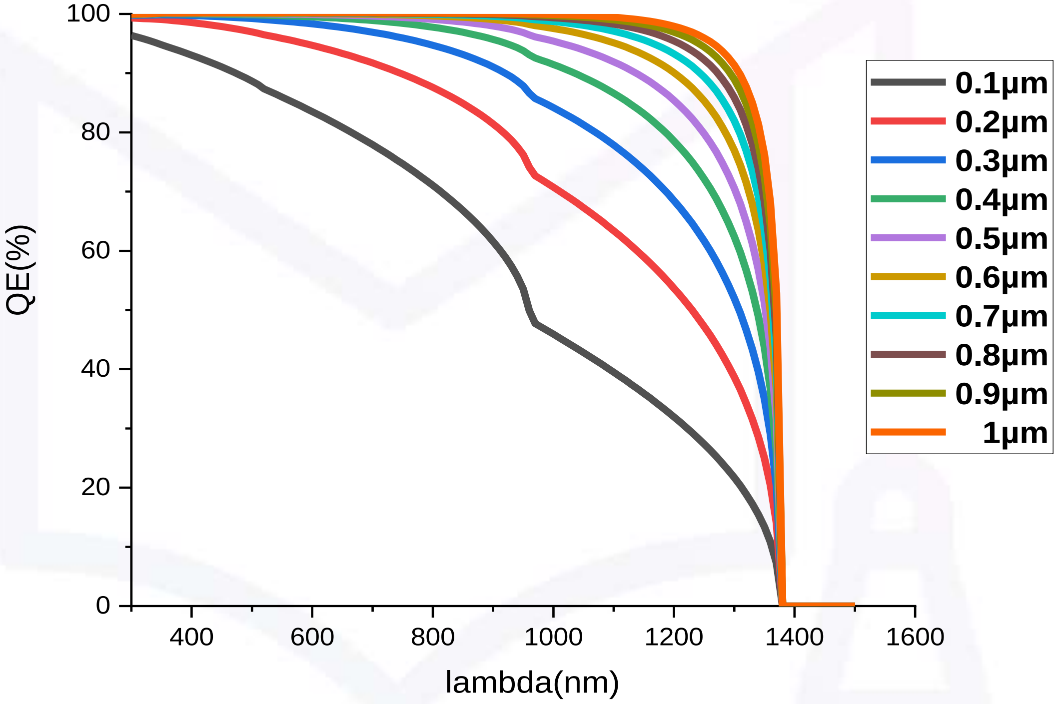

figure (3) :The effect of the thickness of the P-CCZTSe absorbent layer on the quantitative efficiency(QE) curve of the cell WS_2+CCZTSe+CdS+ITO

As shown in the figure(4), the short-circuit current density (J_{SC}) increases as the thickness of the absorption layer (P-CCZTSe) grows from (33.7347355 mA/cm^2) to (51.2192032 mA/cm^2) when thickness (0.1µm) . This is due to an increase in the thickness of the absorbent layer, which produces pairs of electron-hole pairs as photons are absorbed more efficiently[17]. Also, as shown in figure (4), the open circuit voltage (V_{OC}) increases with a small increase from (0.804766 V) when the thickness (0.1µm) to (0.81625 V) when the thickness (1 µm). Increasing the thickness of the absorbing layer leads to the absorption of many photons, which in turn contributes to the production of electron-hole pairs, thus increasing the current and voltage, according to equation (1)[16].

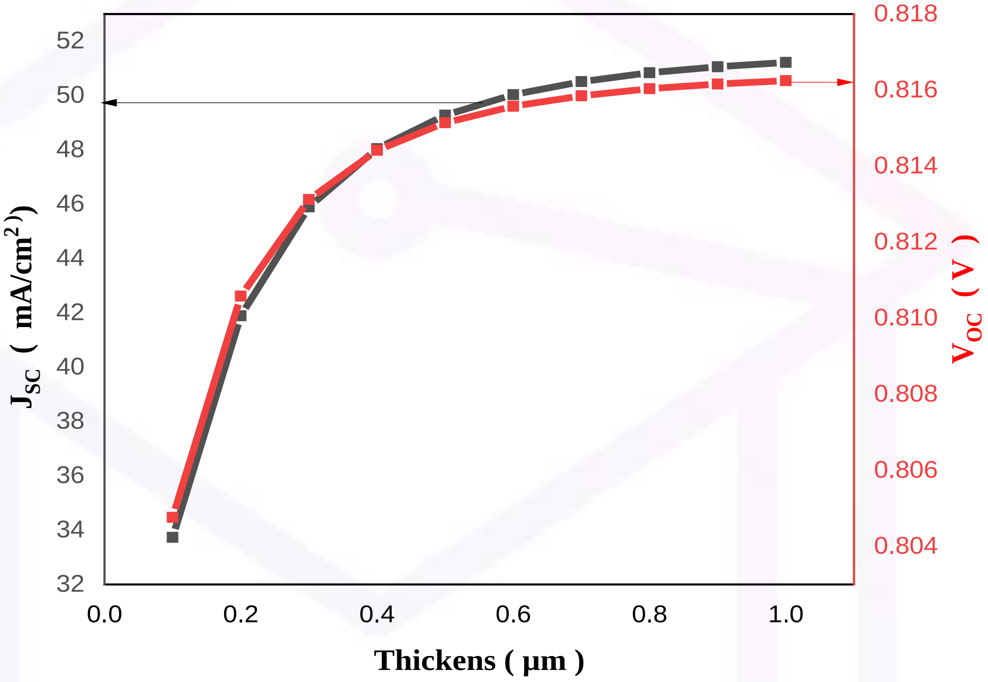

figure (4) :The effect of the thickness of the P-CCZTSe absorbent layer on the short circuit current density (J_{sc}) - open circuit voltage (V_{oc})

In terms of conversion efficiency (Ŋ), it was discovered that when the thickness of the absorbing layer(P-CCZTSe) rose, the efficiency increased as well, starting at (0.1µm) equal (23.2398 %) and ending at (1 µm) (35.8712 %), as shown in the figure (5), The reason for this is to create a voltage barrier between the absorption layer and the back reflection layer, which increases the cell's efficiency because the back reflection layer returns electrons to the other end and prevents them from being collected, reducing the recombination process and thus increasing the cell's efficiency[18]. The filling factor (FF) increases with the thickness of the absorbent layer, but only slightly, thus it goes from (85.6023 %) when the thickness is (0.1µm) to (85.8006 %) when the thickness is (1µm), as shown in the figure (5), However, after an increase, it will decrease due to the

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recombination process, which captures electrons and reduces current, resulting in a decrease in the filling factor, and the filling factor is influenced by the resistance, which has increased in succession as the thickness of the absorbing layer has increased[19].

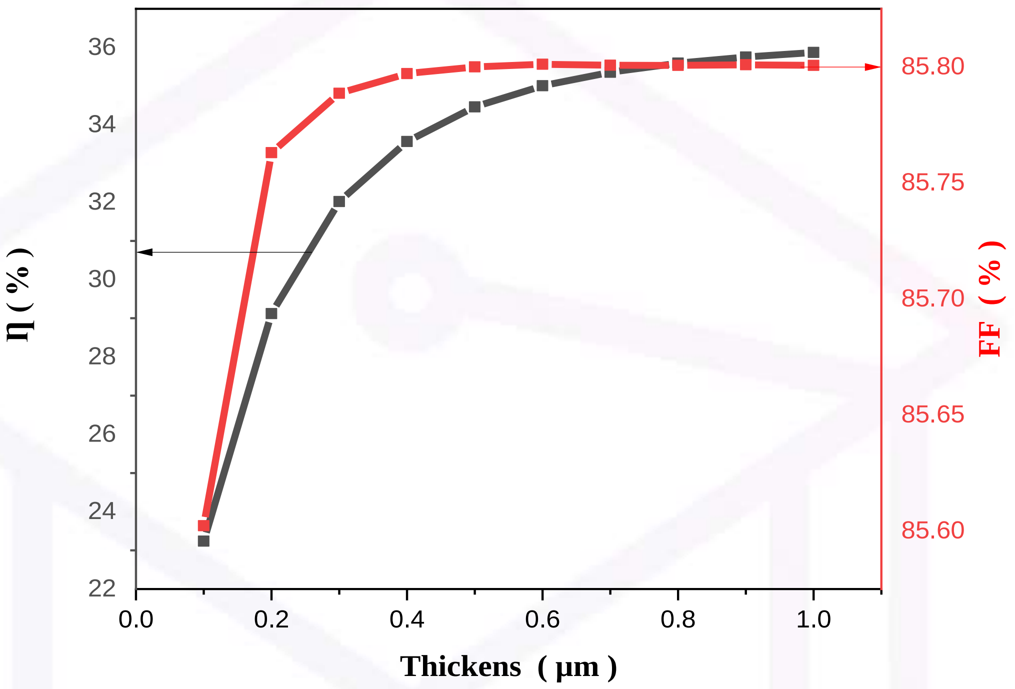

figure (5) :The effect of the thickness of the P-CCZTSe absorbent layer on the conversion efficiency (ŋ) - Fill factor value (FF)

Conclusions

Computer simulation (WS2+CCZTSe+CdS+ITO) was used to simulate photovoltaic cells. Computer simulation (WS2+CCZTSe+CdS+ITO) is a hypothetical program that simulates experimental reality through mathematical equations to suggest cells that are as close to experimental reality as possible at the lowest cost and time. According to the simulation, As shown in table(2), increasing the thickness of the absorbing layer (P- CCZTSe) increased (V_{OC} , J_{SC} , FF , ŋ) respectively (0.804766-0.816250V, 33.7347355-51.21920321 mA/cm^2, 85.6023-85.8006 %, 23.2398-35.8712 %). The increase in the efficiency of the photovoltaic cell is primarily dependent on the back reflection layer (WS_2), which became stable The optical characteristics of the photovoltaic cell improved as the thickness of the absorption layer was raised until it reached about (100 %).

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