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THEME

Study and numerical simulation of photovoltaic cells based on chalcostibite materials

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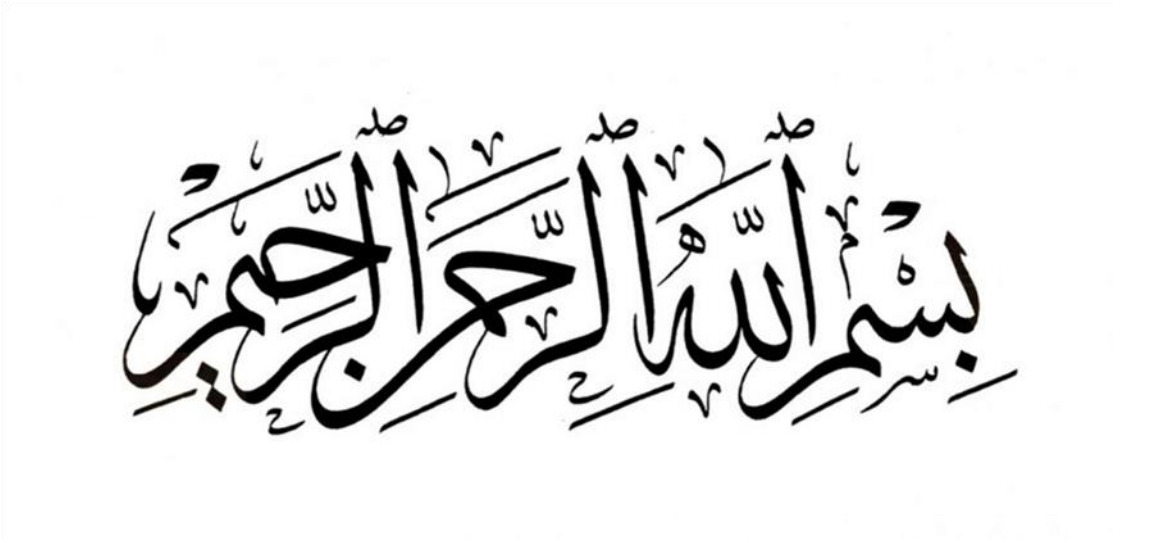
بسم الله الرحمن الرحيم

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I dedicate this humble work:

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Abstract

In this work, by using the wxAMPS-1D package, we have studied and performed a simulation for a thin film solar cell based on Chalcostibite materials ($CuSbS_2$ or $CuSbSe_2$ adopted as an absorber layer), the first proposed solar cell is ZnO/CdS/ $CuSbSe_2$ and the second is ZnO/CdS/ $CuSbS_2$. We have optimized the layers thicknesses and doping concentrations in order to improve the photovoltaic performance of these solar cells, the obtained maximum efficiencies are 14.19 % and 18.84 %, for $CuSbSe_2$ and $CuSbS_2$ based solar cells, respectively.

Keywords: solar cells, Chalcostibite, CuSbS2, $CuSbSe_2$, simulation, wxAMPS-1D.

Résume

Dans ce travail, en utilisant le logiciel wxAMPS-1D, nous avons étudié et procédé une simulation pour une cellule solaire à couche mince basée sur des matériaux Chalcostibites ($CuSbS_2$ ou $CuSbSe_2$ adoptés comme couche absorbante), la première cellule solaire proposée est ZnO/CdS/$CuSbSe_2$ et la seconde est ZnO/CdS/$CuSbS_2$. Nous avons optimisé les épaisseurs de couches et les concentrations de dopage afin d'améliorer la performance photovoltaïque de ces cellules solaires, les efficacités maximales obtenues sont de 14,19 % et 18,84 %, pour les cellules solaires à base de CuSbSe2 et CuSbS2, respectivement.

Mots clés: cellule solaire, Chalcostibite, CuSbS2, $CuSbSe_2$, simulation, wxAMPS-1D.

ملخص

في هذا العمل، باستخدام برنامج wxAMPS-1D، قمنا بدراسة وإجراء محاكاة لخلية شمسية رقيقة تعتمد على مواد الكالكوستيبايت ($CuSbS_2$ أو $CuSbSe_2$ تم اعتمادها كطبقة ممتصة)، أول خلية شمسية مقترحة هي ZnO/CdS/ $CuSbSe_2$ والثانية هي ZnO/CdS/ $CuSbS_2$. لقد قمنا بتحسين سمك الطبقات وتركيزات الإشابة (التطعيم) من أجل تحسين الأداء الكهروضوئي لهذه الخلايا الشمسية، وتبلغ كفاءة الخلايا الشمسية التي تم الحصول عليها 14.19٪ و 18.84٪ للخلية الشمسية $CuSbSe_2$ و $CuSbS_2$، على التوالي.

الكلمات المفتاحية الخلايا الشمسية، الكالكوستيبايت، $CuSbSe_2$ ،CuSbS2، محاكاة، wxAMPS-1D .

Summary

Chapter I: An overview on Chalcostibites Materials.

Chapter II: An overview on photovoltaic cells.

Chapter III: Results and Discussion.

List of figures

List of tables

List of Symbols and Abbreviations

Symboles	Meaning	unity
α	The absorption coefficient	cm^{-1}
Eg	Forbidden Band Energy	eV
R_s	Resistance Series	Ω
R_p	Parallel resistance	Ω
I_{PH}	The photo-current	mA
d_1, d_2	diode	V
V	voltage	V
I	The current	A
Vj	the positive current	V
Is_1	saturation in progress	A
q	the elemental load (1.6 x10 -19 C)	C
n	Densities of free electrons	cm^{-3}
K	Boltzmann constant (1.38 x10 -23 J.K-1)	$J.K^{-1}$
T	absolute temperature	K
I_S	saturation current	A
I_{sc}	The current of a circuit breaker	mA/cm^2
V_{oc}	The tension in an open circuit	V
P_{max}	The power supplied to the external circuit	W
I_{max}	Density of current at the maximum power point	A
FF	the filling factor	%
η	The Efficiency	%
h	Planck constant (6.62 x 10 -34 J.s)	J.s
v	The frequency of the incident radiation	s^{-1}
J_0	The saturation current density	mA/cm^2
Jcc (JSC)	Short circuit current density (short circuit)	mA/cm^2
Nc	The density of equivalent states in the BC, reduced to Ec	cm^{-3}
Nv	The density of equivalent states in the BV Ev	cm^{-3}
N_a	Concentration acceptor	cm^{-3}
N_d	Concentration of donor	cm^{-3}
u_n	The mobility of electrons	$cm^2.V^{-1}.S^{-1}$
u_p	The mobility of holes	$cm^2.V^{-1}.S^{-1}$
E_c	Energy from the bottom of the conduction band	J ou eV
E_v	Energy from the top of the valence band	J ou eV
E_F	The Fermi energy	eV

General Introduction

The rapid increase in global energy demand, the rise in fossil fuel prices, the increase in global pollution, global climate change and the demand to reduce CO_2 emissions from the earth's atmosphere have highlighted the need for a sustainable supply of renewable energies. Photovoltaic (PV) generation is a sustainable renewable energy source and currently, it represents one of the largest absolute generation growths of all renewable technologies. In 2019, the global solar PV module market size was estimated at $115.2 billion dollar and it is expected to grow at rate of 4.3% from 2020 to 2027 [1]. Among all types of solar PV panels the market share of thin film solar PV panels are around 40.0% in 2019 [1]. However the contribution of solar PV is still low compared to the global demand of energy, and the current PV technologies face some challenges in ramping up total PV manufacturing to the terawatt per year level [2].

Silicon is the most important commercialized PV material with a market share of more than 90% in the single-crystal (c-Si) and multicrystalline (poly-Si) forms [3]. Even so silicon is an indirect semiconductor and therefore a relatively thick layer is required to absorb the incident light. In addition, the high raw material and processing costs make silicon expensive in itself. And in principle, other materials might be better suited for long-term PV production [2].

Alternatives have emerged in recent years, notably direct semiconductor-based thin-film solar technologies that require only a few microns to absorb light and can be processed at relatively low temperatures [2]. The two most important are cadmium telluride (CdTe) and copper indium gallium diselenide (CIGS), with laboratory efficiencies in excess of 20% [4]. The main limitations to expanding CdTe solar cell manufacturing are the toxicity of Cadmium and the scarcity of Tellurium [5].CIGS thin films are essentially limited by the high cost of Indium and Gallium [6]. Also amorphous silicon (a-Si) is an unstable material and its efficiency in PV devices is low [2]. These considerations have led to increased interest in emerging light-absorber materials with less toxic and more abundant elements, including Cu_2SnS_3 (CTS), Cu_2O, Sb_2Se_3, Cu_3N, SnS,$ZnSnN_2$, and $Cu_2ZnSn(S,Se)_4$ (CZTSSe). Among these, the highest PV efficiency (certified 12.6%) has been reported for the CZTSSe absorber [7]. However, its further improvements may be hindered by chemical and crystallographic complexity, pointing researchers toward less complex materials [7].

Considerable attention has recently been paid to thin-film solar cells based on high-efficiency absorbers due to their applicability in flexible photovoltaic technology. Hence, thin-film solar cells with Earth-abundant and nontoxic materials need to be investigated as possible candidates. Toward this goal, different compounds of $CuSbSe_2$, $CuSbS_2$, $CuBiS_2$ and $CuBiSe_2$ are being considered as potential low-cost sustainable absorber materials for inorganic thin-film solar cells [8].

The main objective of this work is to study the influence of some physical properties, such as: the thickness of the absorber and the doping concentrations, on the photovoltaic performance of the solar cells, With the ZnO as a window layer and the CdS as a buffer layer, $CuSbS_2$ and $CuSbSe_2$ adopted as an absorber layer. We will use the simulation tool wxAMPS-1D to optimize the thickness values and the doping concentrations for each layer of the proposed solar cells. Our work structure is given as follows:

After a general introduction, the first chapter contains a definition of the proposed compounds and their optical and electrical properties in addition to their crystal structure.

The second chapter describes general information on the photovoltaic solar cells, the principle of operation and their types, as well as the advantages and disadvantages of these solar cells.

In the third chapter, we will present the wxAMPS-1D package used in our simulation study, also discussions and interpretations of the results obtained by simulating our proposed solar cells.

Finally a general conclusion resumes the obtained results and the perspectives of the work.

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CHAPTER I

An overview on Chalcostibites Materials

I.1. Introduction

The world energy demand is growing very rapidly, the accelerated increase of the energy consumption had a dramatic impact on the global warming rate last century and can have catastrophic and irreversible repercussions on the climate. In order to solve this problem, the expansion of renewable energy sources will play a key role the following decades. Among the renewable energies, solar photovoltaics (PV) is growing very fast, however the contribution of solar PV is still low compared to the global demand of energy, and the current commercialized PV technologies face some challenges in ramping up total PV manufacturing, so the PV research community is given attention to the development of thin film solar cells. As we can see the most widely studied materials for thin film solar cells are $Cu(In,Ga)Se_2$ (CIGS, 23.4% one sun energy conversion efficiency) and CdTe (23.2% efficiency) [1] Nonetheless, the future environmental benefits and the potential scope of use of these solar cells may be limited by their elemental scarcity (In, Ga, Te) and toxicity (Cd). Quaternary compounds Cu_2-II-IV-VI_4 represented by Cu_2ZnSnS_4 or $Cu_2ZnSnSe_4$ have been proposed to replace the deficient and expensive elements mentioned above. Up to 13.0% [1] (theoretical 23.67%, [2]) of the energy conversion efficiency has been achieved, but difficulties still remain in controlling the composition and morphology in the quaternary compound. Thin-film solar cells with Earth-abundant and nontoxic materials (chalcostibite) need to be investigated as possible candidates toward this goal, different compounds of $CuSb(SSe)_2$ and $CuBi(SSe)_2$ are being considered as potential low-cost sustainable absorber materials for inorganic thin-film solar cells.[3,4].

Chalcostibite have shown great promise as alternative absorber materials for cost-effective photovoltaic energy production [3].This is a result of their high absorption coefficients, optimal band gap, and consist of cheap, low-toxic, and earth-abundant elements. Among these semiconductor materials we have the chalcostibite $CuSb(SSe)_2$ which broadly used in recent years in high efficiency solar cells fabrication [5].Due to their high absorption coefficients, that are over 10^5 cm^{-1}, band gaps in the range between 1.1 and 1.8 eV [5].

Ternary copper bismuth sulfides $CuBi(SSe)_2$ have been investigated in recent years as an absorber material for inexpensive photovoltaic energy generation. Because of their high absorption coefficients (>10^5 cm^{-1}), optimum band gap (~1.4-1.7 eV) [5] and consist of cheap, low-toxicity and earth-abundant elements.

In this chapter, we will present the crystal structure and the optoelectronic properties of these compounds.

I.2. physical properties

I.2.1. Crystal structure

Ternary $Cu(Sb,Bi)(SSe)_2$ compounds crystallize in orthorhombic structure (Pnma space group no. 62) [6]. The cations Sb/Bi are four-coordinated while Cu atoms are five-coordinated with respect to the neighboring anions S or Se [7]. Fig (I.1) shows the crystal structure of these compounds. Left panel represents the normal bonding arrangement while right panel shows the polyhedral configuration.

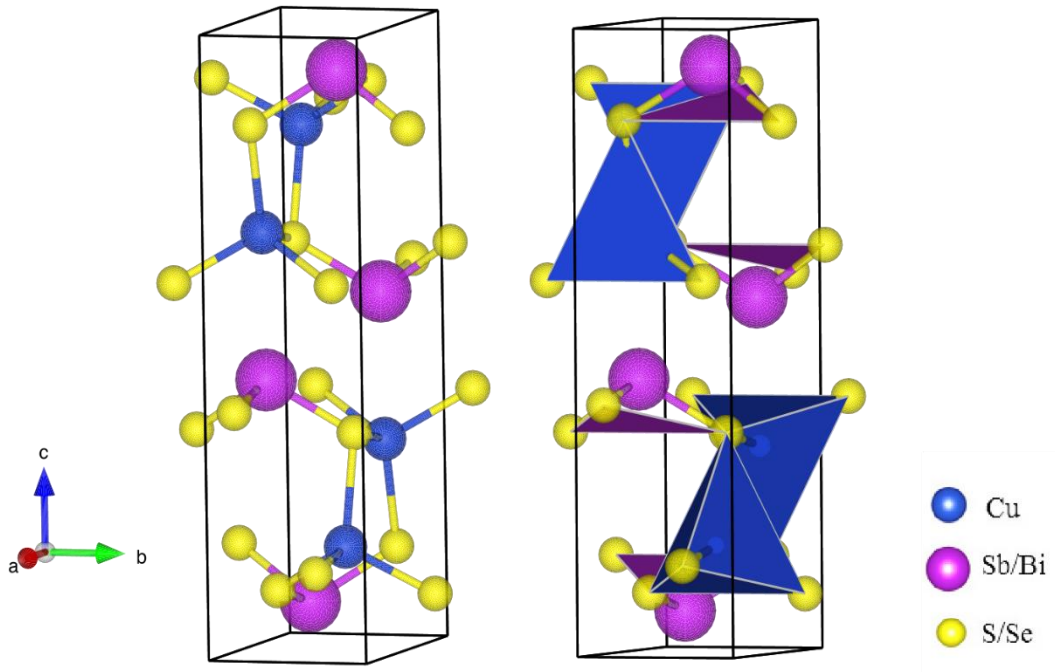

Fig.I.1. The crystallographic structure of the $Cu(Sb,Bi)(S,Se)_2$ compounds [7].

The unit cell with 4 Cu atoms, 4 Sb/Bi atoms, and 8 anions (S or Se) contains 16 atoms and these atoms occupy 4c Wyckoff sites [7]. The lattice parameters (a, b, and c) of these compounds are shown in Table (I.1).

Table.I.1. The lattice parameters (*a*, *b*, and *c*) of the Ternary Cu (Sb,Bi)$(SSe)_2$ compounds [7].

	$CuSbS_2$	**$CuSbSe_2$**	**$CuBiS_2$**	**$CuBiSe_2$**
a (A^0)	6.05(6.014)[a]	6.43(6.299)[a]	6.18(6.134)[b]	6.58
b (A^0)	3.81(3.788)[a]	3.95(3.973)[a]	3.93(3.911)[b]	4.11
c (A^0)	14.55(14.472)[a]	15.35(15.005)[a]	14.64(14.548)[b]	15.05

The most absorbers used in solar cells have a tetrahedrally bonded lattice, where different atoms are linked to one another in 3D diamond structures like (Si, CdTe, $CuInS_2$, and Cu_2ZnSnS_4). However, the Chalcostibites shows a very different 2D-like layered crystal structure. Fig (I.2) shows the crystal structure of the chalcostibite (b) compared to the structure of the chalcopyrite $CuInS_2$ (a) [8].

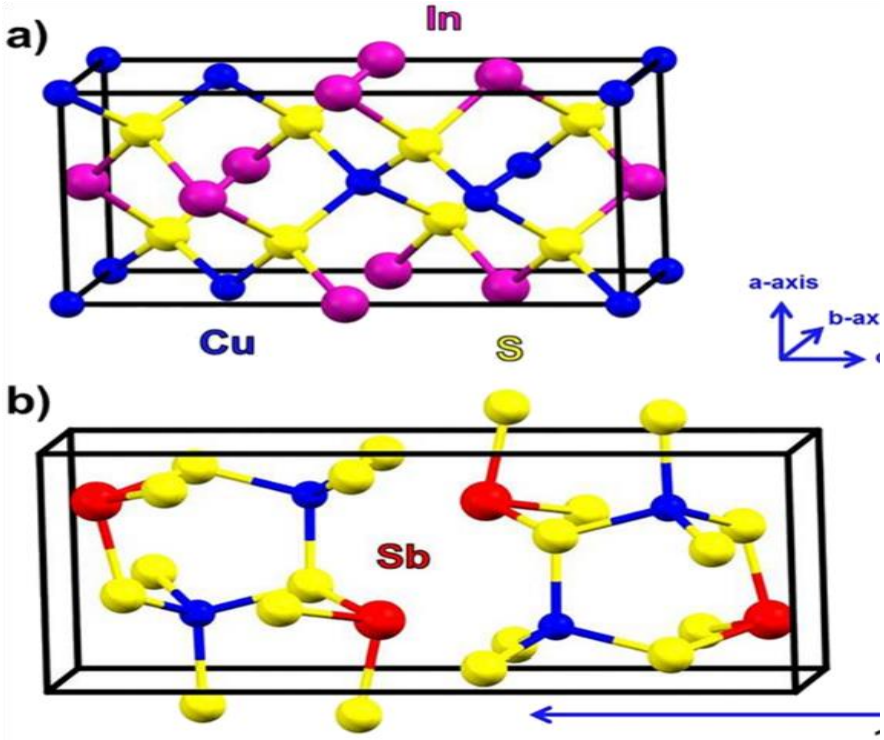

Fig.I.2. The crystal structure of (a) Chalcopyrite $CuInS_2$ (b) chalcostibite [8].

I.2.2. Optical properties

One of the most important parameters in the choice of the PV materials is the absorption coefficient α (ω) which is shown in Fig (I. 3) for the $Cu(Sb,Bi)(SSe)_2$ [7].

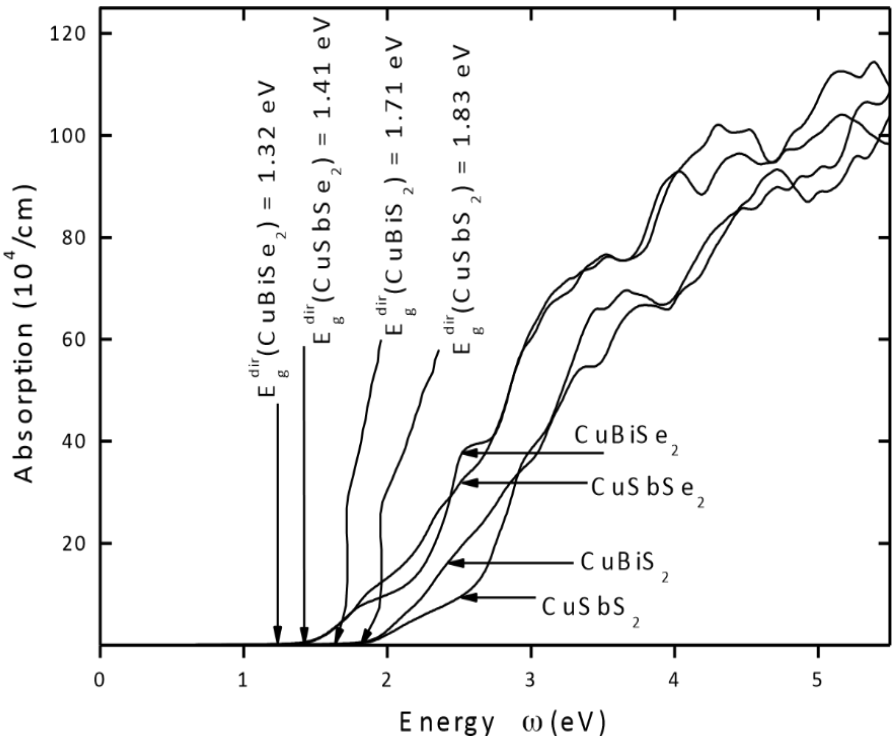

Fig.I.3. The absorption coefficients α(ω) of $Cu(Sb,Bi)(S,Se)_2$ compounds **[**7].

It is clear from Fig (I.3) [7] that the optical absorption of these compounds is large (over 10^5 cm^{-1} [5]) and suitable for PV applications. *Mukesh Kumar and Clas Pesrsson* [7] have compared the absorption coefficients of the chalcostibites with the well-established compounds $CuInS_2$, and $CuInSe_2$ (Fig.I.4).

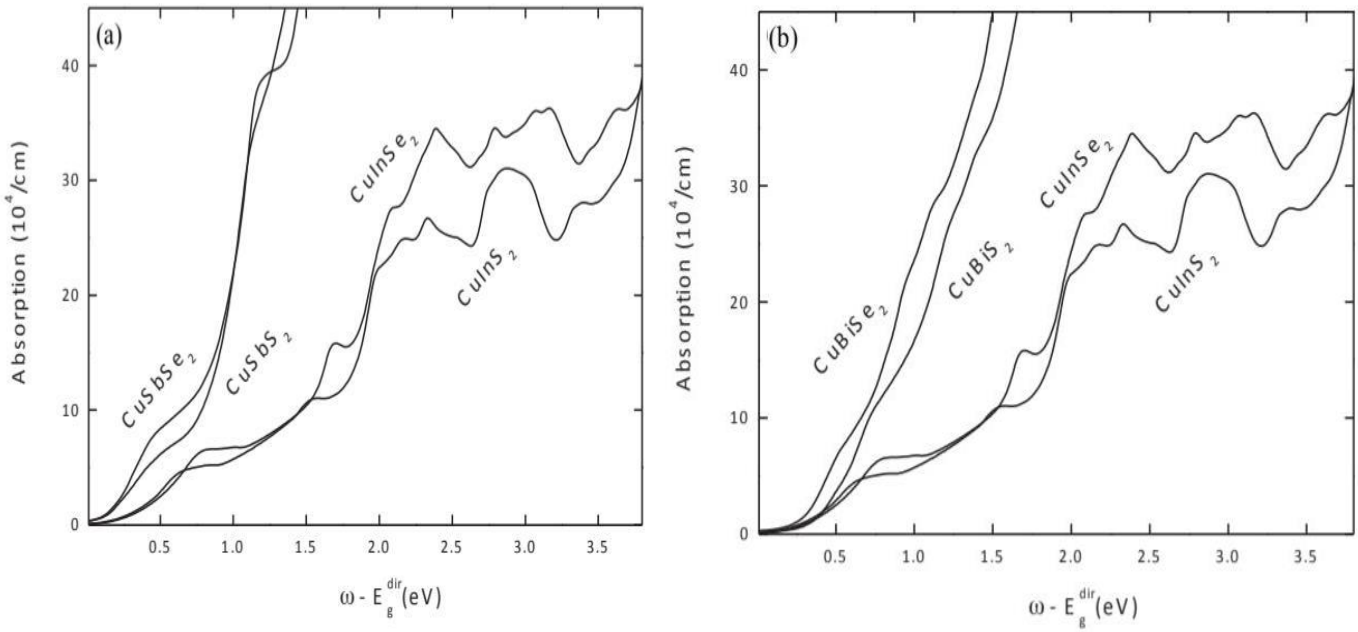

Fig.I.4. The absorption spectra of (a) $CuSbS_2$, $CuSbSe_2$ and (b) $CuBiS_2$ $CuBiSe_2$ are compared with the chalcopyrites $CuInS(Se)_2$ [7].

The absorption coefficients of Cu (Sb, Bi)$(SSe)_2$ compounds are about twice as large as in the conventional Cu-based chalcopyrite. Overall, all these compounds have large absorption coefficient and the reason for this is related to their electronic structure [7].

I.2.3. Electronic band structure

The band gap of these semiconductors is represented in the fig (I.5) where The VB Maximum is located along the line between Γ-point and Z-point, while the CB minimum is in U-R-S-X-Γ Region, also the electronic band structures of Cu (Sb, Bi)$(SSe)_2$ compounds demonstrate that these compounds have flat CBs and indirect band gaps and the fundamental band gap energies are 1.72, 1.36, 1.58, and 1.14 eV for $CuSbS_2$, $CuSbSe_2$, $CuBiS_2$, and $CuBiSe_2$, respectively [7].

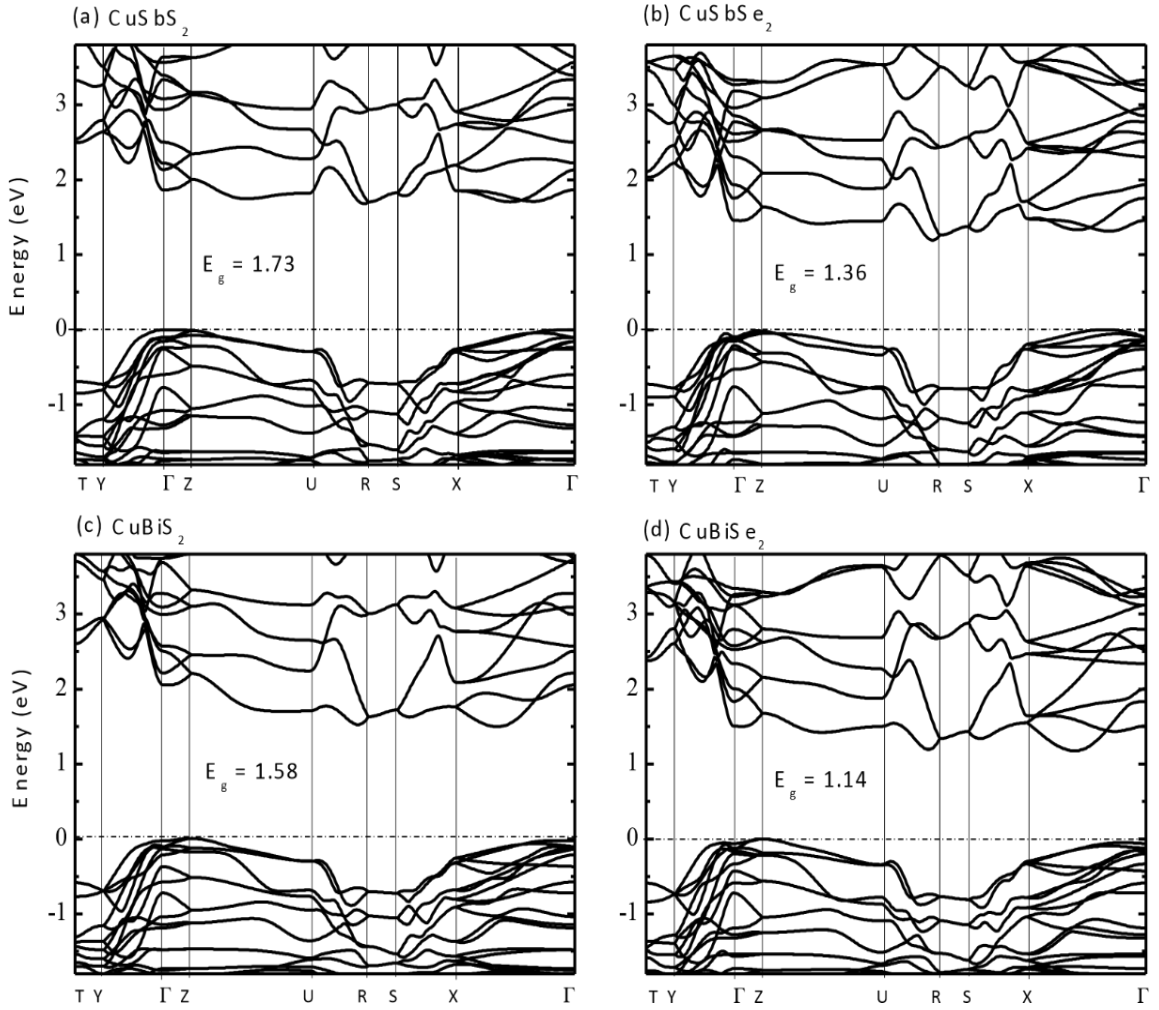

Fig.I.5. The electronic band structure of (a) $CuSbS_2$ and (b) $CuSbSe_2$ (c) $CuBiS_2$ (d) $CuBiSe_2$ [7].

I.3. Conclusion

To summarize, $Cu(Sb,Bi)(SSe)_2$ compounds are orthorhombic semiconductors made up of relatively cheap and plentiful elements. $CuSbS_2$, $CuSbSe_2$, $CuBiS_2$, and $CuSbSe_2$ exhibit indirect band gaps of 1.72, 1.36, 1.58, and 1.14 eV, respectively. Furthermore, from references, these compounds have strong optical absorption compared to chalcopyrite $CuIn(SSe)_2$ and all these compounds have large absorption coefficient, and that's making it the material of choice for new thin film solar cells.

I.4. References

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CHAPTER II

An overview on photovoltaic cells

II.1.Introduction

Solar energy can be defined as the heat and light coming from the sun, which man has used in his service since ancient times, through the use of some of the most advanced and traditional means of technology. Due to their advantages photovoltaic energy plays a significant role among these advantages are the following photovoltaic technology has environmental benefits because the final product is non-polluting, quiet, requires little maintenance, has no additional electrical lines, solar cells do not contain mobile parts, making them particularly suitable for isolated areas, this is the reason for its widespread use aboard spacecraft, as well as its high reliability most manufacturers guarantee their modules for a period of 25 years, on the other hand, photovoltaic energy has some drawbacks, such as photovoltaic module manufacturing requires advanced technology and high-cost investments; photovoltaic module manufacturing requires high-cost investments the actual conversion rate of a module is low finally when storing electrical energy in chemical form (batteries) is required the cost of a photovoltaic generator rises [1]. The research has begun on the development of promising techniques for recovering this energy which are based on the properties of semi-conductors. The thin film solar cells are one of the several photovoltaic technology available [2], as the CIGS (cuivre, indium, gallium, and selenium) and CdTe (cadmium telluride). However, these thin films contain toxic and rare elements. [3] In this context the $CuSbSe_2$ and $CuSbS_2$ are promising candidates to replace the CIGS and CdTe in photovoltaic thin-film applications [4].

In our study we will focus on materials that are widely abundant in nature and at a low price called chalcostibite.

II.2. Photovoltaic solar cells

Among the renewable energy sources, solar energy is the most promising and powerful photovoltaic (PV) electricity is generated by converting direct sunlight into electricity using PV cells. The term photovoltaic comes from the Greek word photon, which means light. Edmond Becquerel a French physician discovered it in 1839. The photovoltaic effect is the direct conversion of solar radiation into electrical energy of a continuous type that may be used directly through solar cells [5]. The principle behind this phenomenon is a semi-conductor contains two regions one with an excess of electrons and the other with a deficit of electrons,

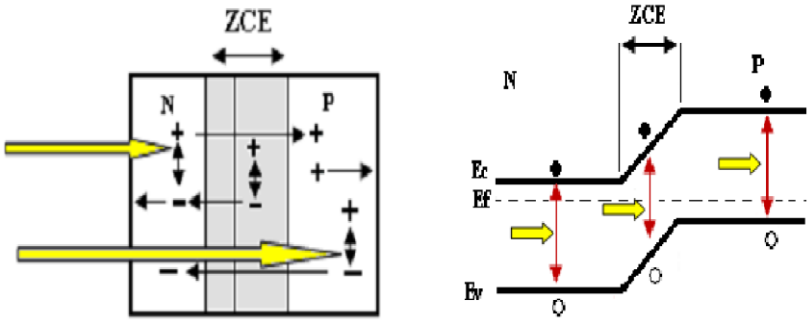
referred to as doped n and doped p, respectively when the first comes into touch with the second, the excess electrons in the type n material diffuse into the type p material. The first doped zone n becomes positively charged while the initially doped zone p becomes negatively charged. As a result, an electric field is formed between them, which tends to keep the electrons in zone n and the holes in zone p, forming a diode.

II.2.2.1. Principle of photovoltaic cell

The solar cell is a large-area photodiode with PN junctions that generates an electrical signal without the use of an external energy source. When photons enter the cell, some are reflected while others are transmitted or absorbed, only the photons that are absorbed participate in the photovoltaic effect. Three physical phenomena, inextricably linked and occurring at the same time are involved in photovoltaic conversion [6]:

- Absorption of photon (whose energy is greater than the gap) by the material that makes up the device.
- Conversion of photon energy to electrical energy, resulting in the formation of electron/ hole in semi conductive materials.
- Collects particles generated by the device.

As a result, it is clear that the materials that make up a solar cell must have specific optical and electrical properties in order to allow photovoltaic conversion. In order to gather the generated electron- hole, an electrical field capable of dissociating the created electron- hole is required. For this, the most common configuration is a PN junction. Figure (II.2) illustrates the operation of photovoltaic cell.



(a) (b)

Fig.II.1. Structure (a) and band diagram (b) of a photovoltaic cell [7].

Depending on the region, the generated electron- hole behaves differently:

- Minoritarian carriers disperse in the N and P zones. What reaches the space discharge zone is propelled by the electric field toward zone P (for the holes) and zone N (for the electrons), where they will be the majority. This photo-courant of diffusion is caused by the transport of charge carriers.
- The photon-hole pairs generated in the space charge zone will be directed by the electric field to the region N (electron) and P (photon) (hole). These two contributions together have the result of giving a total I_{PH} (photo current) it's a current of minority carriers. It is proportional to the light intensity [8].

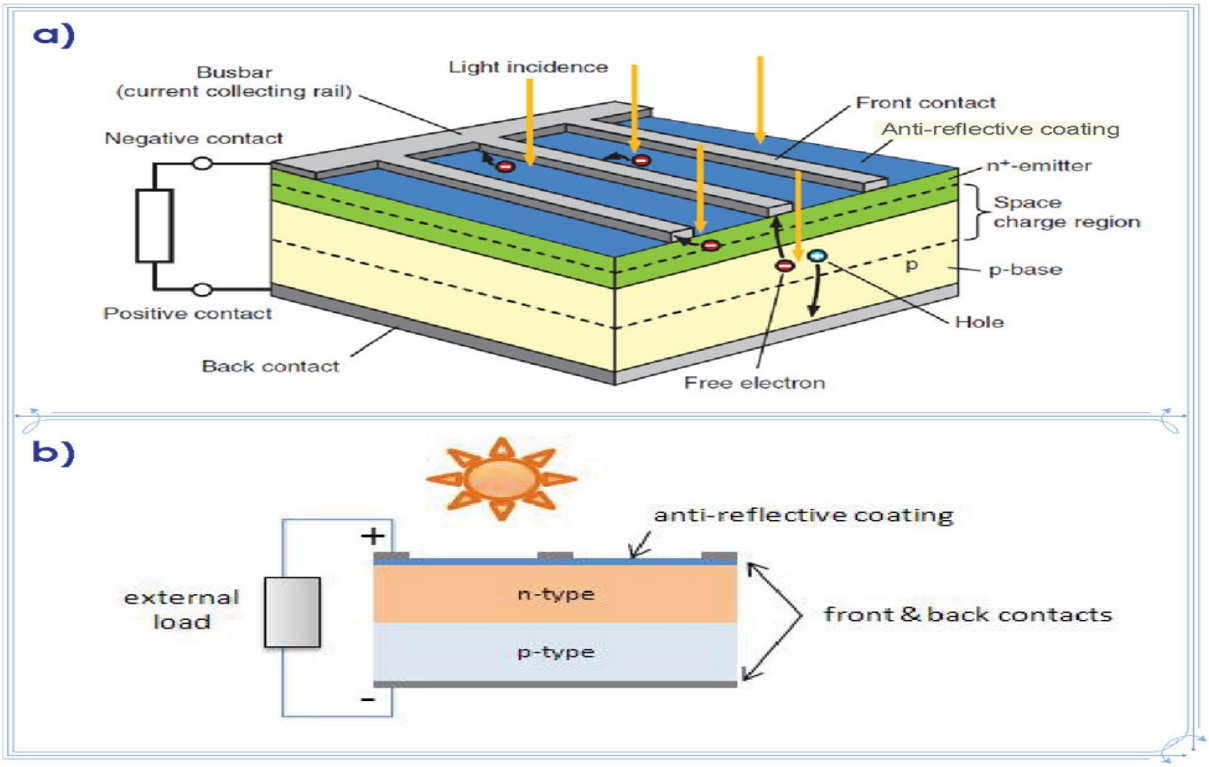


Fig.II.2. A snapshot on conventional solar cell featuring front and back contacts. [9].

II.2.3. Electrical model of a photovoltaic cell

The (figure II.3) proposes a double diode electrical model of a photovoltaic cell that takes into account various limiting factors. The current generator I_{ph} corresponds to the photo-generated current, as well as additional resistances (R_S and R_P), two diodes (d1, d2), and the charge resistance R_c [10].

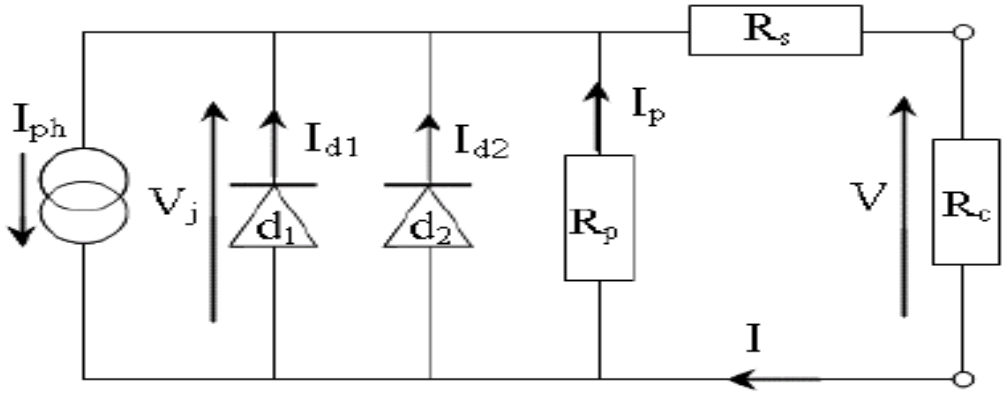


Fig II.3. Double diode equivalent circuit of a photovoltaic cell [10].

- **Current generator:** It generates the current I_{ph} that corresponds to the current photo.
- **R_S Resistance Series**: It considers the specific resistance of the contact between the various regions of the cell (that is, the electrode, the base, and the metal contacts). Ideally, this term should be as short as feasible in order to have the least impact on the cell's current. This can be accomplished by optimizing the metal-to-semiconductor contact. And by lowering the resistance of the materials used. A high dose on the other hand causes an increase in porter recombination.
- **Parallel R_P resistance:** She is also known as short circuit resistance, and it indicates the presence of shunts in the emitter due to a fault. This is the case when the emitter detects the diffusion of metal connections at high temperatures. It could also be caused by a short circuit at the cell's edges. This value should be as high as feasible.
- **D1 diode**: Models the distribution of porters in the base and the emitter. His influence will be greater if the material has a sufficient length of diffusion.

- **D2 diode**: Models the generation and recombination of porters in the space charge zone.

$$I(v) = I_{PH} - I_{D1} - I_{D2} - V_g/R_P \quad (II.1)$$

$$I_{PH} - I_{S1}[\exp(\alpha_1 - V_J) - 1] - I_{s2}[\exp(\alpha_2 V_j) - 1] - V_J/R_P \quad (II.2)$$

Combined with:

$V_J = V + I.R_S$ (In the case where the curve (I-V) is represented in the positive current and voltage);

I_{PH} : a photo-generation course;

I_{D1} : In the space charge zone, there is a recombination generator or a tunnel effect.

I_{D2} : a diffusion path through neutral zones;

R_P : Parallel resistance;

R_S : series of resistance;

I_{S1} : saturation in progress;

$\alpha = q/nKT$ with n: the diode's ideality factor.

II.2.4. The electrical parameters of solar cell

A solar cell consists of a PN junction, the latter made from materials sensitive to light, it has the particularity of being able to operate in photovoltaic generator. This static behavior can be described by equation (II.3) defining the behavior of a diode under illumination [11] [12].

$$I = I_{obs} - I_{ph} = I_s(\exp(qV/nkT) - 1) - I_{ph} \quad (II.3)$$

This relationship between the three magnitudes, I, I_{PH}, and I_{obs} (V), represents the Perfect current tension characteristic for determining the main characteristic quantities of the

Operation of solar cells:

- I_{sc} : The current of a circuit breaker.
- V_{oc} : The tension in an open circuit.

- P_{max} : The photodiode's maximum capacity is deducted.
- I_{max} : Density of current at the maximum power point.
- V_{max} : Maximum tension pressure.
- FF : The shape-shifting factor.
- η : The rate of energy conversion [11] [13] [14].

II.2.4.1. Short circuit current, I_{sc}

This is the current obtained at the cell terminals when the voltage at these terminals is zero, It is the maximum current that can be obtained from a cell. Its typical value will be about 10 mA/cm^2. If $R_s << R_p$ is present, $I_{sc} = I_{ph}$ can be used [15] [16].

II.2.4.2. Tension in an open circuit V_{oc}

This is the voltage for which the current at the cell terminals is zero; it is the maximum voltage that can be obtained from a cell; it is around 0.6 V for the cell silicon. It is obtained from equation (I.4) for I=0 and VT=KT/q as the thermal potential, the expression for V_{oc} is as follows [16] [17]:

$$I = I_{sc} - I_s(\exp(q(V + IR_s)/nKT) - 1) - (V + IRs/R_p) \quad (II.4)$$

$$V_{oc} = KT/q \ln(I_{sc}/I_s + 1) = V_t \ln(I_{sc}/I_s + 1) \quad (II.5)$$

II.2.4.3. The maximum power point P_{max}

The power supplied to the external circuit by a photovoltaic cell under illumination depends on the load resistance (external resistance placed at the terminals of the cell). This power is maximum (rated P_{max}) for a P_{max} operating point (I_{max},V_{max}). The maximum P_{max} can be determined by plotting the characteristic IV and constant-power hyperboles on the same graph. The optimal point of operation corresponds to the point of tangence of two curves, as shown in Figure (II-4). [11] [18] [19]:

The maximum power delivered to the charge is given by the expression (II.6):

$$P_{max} = V_{max} . I_{max} \quad (II.6)$$

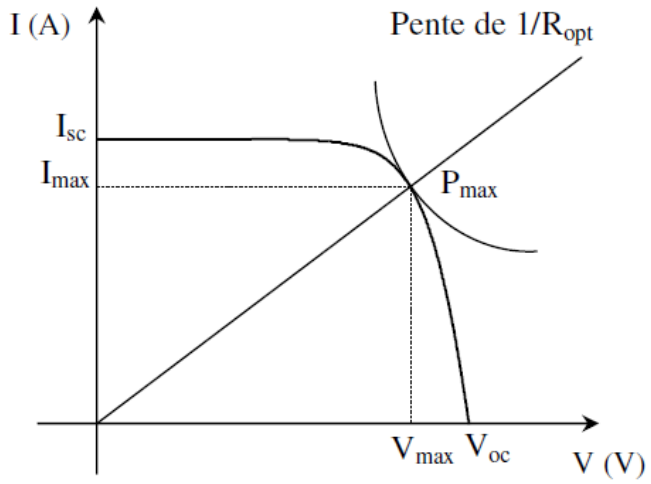


Fig. II.4. Maximum power point of a single atomic cell [19].

II.2.4.4 Fill factor (FF)

An important parameter is often used from characteristic I(V) to qualify the quality of a cell or a PV generator: it is the filling factor (FF), this coefficient represents the ratio between the maximum power delivered by the cell rated P_{max} and the power formed by the rectangle $I_{sc}.V_{oc}$. It is of the order of 0.7 for the performance cells; and decreases with temperature, their expression is given by [12] [18] [20] [21]:

$$FF = \frac{PMAX}{Isc.Voc} = \frac{Vmax.Imax}{Isc.Voc} \qquad (II.7)$$

II.2.4.5. The Efficiency (η)

The Efficiency of a photovoltaic cell is the ratio of converting luminous energy into electrical energy, which is equal to the ratio of the maximum output power to the power of luminous radiation. This is the criterion that determines how well a PV cell performs, and it is determined by:

$$\eta = \frac{Pmax}{Pin} = \frac{Vmax\ Imax}{Pin} = \frac{Voc\ Isc\ FF}{E\ S} \qquad (II.8)$$

Where P_{in} is the input power that is clearly incident on the PV cell per unit of surface, corresponding to the clearly luminescent E of the sun in the form of photons per unit of surface received (at standard conditions, 1000W/ m^2), S is the cell's surface, and FF is the fill factor. [15] [14], [22], and [16], respectively.

As can be seen, the efficiency of a solar cell's power conversion is proportional to three key photovoltaic parameters: the short-circuit current I_{sc}, the open-circuit voltage V_{oc}, and the factor of filling FF, for a clearly defined E [21].

II.2.5. Criteria for choosing photovoltaic materials

A brief overview of the properties of materials (usually semiconductors) concerning the functioning of solar cells is given under this title. A number of Properties are required for PVS materials and solar cell structure, the most essential, regarding photonic conditions (optoelectronics and electrical) [23].

1. Due to the quantitative condition hv > Eg. The size of the restricted band, for example, influences the material selection. The greater the number of photons that may be used, the lower the Eg, but the lower the photo-tension. The calculations show that the best Conversion η results will be obtained if Eg is between 1 and 1, 7 eV, as shown in figure (II.10) [24, 25, 26]

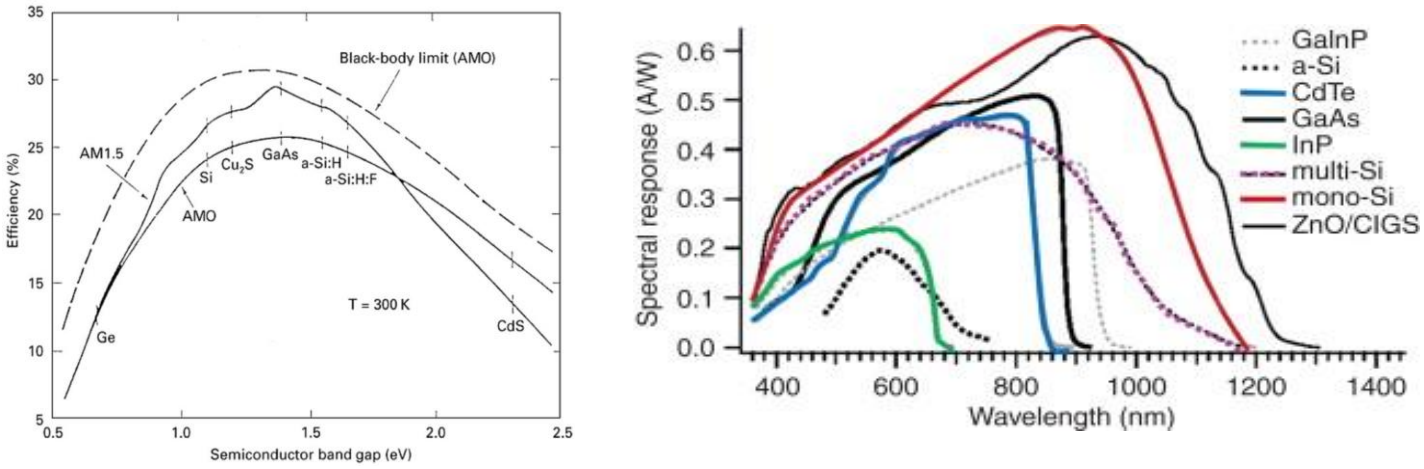


Fig.II.5. The ideal conversion efficiency variation for a cell as a function of the forbidden band width of the material (left) [27]. And the spectral variations of the sensitivity of a solar cell to (Si) or (GaAs) (right). RQI stands for internal quantitative performance [28].

2. Absorption of light over a broad spectral range, particularly in the visible range of the solar spectrum. This property implies that the energy gap is optimal (tunable and desirable).For maximum efficiency, the absorption peak should be [1.4-1.5] eV [29, 30].
3. Low reflectance [31].
4. To make efficient solar cells, the materials utilized must have excellent minority and majority carrier collection capabilities [24-25, 32-30].
5. Low carrier recombination loss (carrier) [25, 32-30].
6. To ensure large-scale production, it must be plentiful and available in sufficient amounts [25].
7. Inexpensive, non-toxic, and environmentally friendly [24, 25].
8. Stability as a function of time and environmental circumstances (corrosion resistance, for example) [24, 25].

II.2.6. Generations, Materials and technologies of solar cells

Photovoltaic cells are divided into a number of categories. The design materials used, the manufacturing process, and the number of connections employed in the cell all varied. The progressive increase in the efficiency over time is depicted in Figure (II.6).

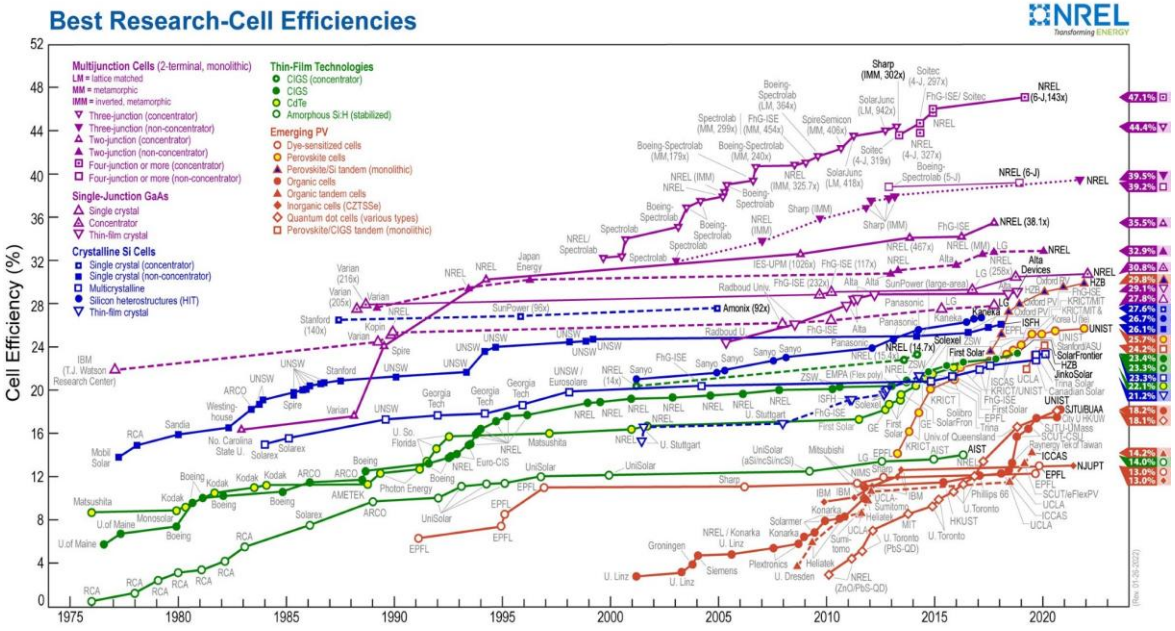


Fig.II.6. Best records PV cells efficiencies chart from 1975 until now [33].

The journey of manufacturing processes of solar cells has seen numerous transformations starting from the first Generation Solar Cells (Wafer Silicon Based), these cells can also be recognized as conventional/ traditional solar cells which are fabricated on thin silicon layers called wafers. And they are classified into Monocrystalline Solar cells and Polycrystalline Silicon Solar cells [34].These cells are chemically stable, have negligible defects. Initially, the power conversion rates of these cells were found to be $17\% - 18\%$ [35] which further enhanced up to 27.6% [36]. Major drawback of these cells is that these cells do not operate efficiently whenever the ambient temperature rises above $25^{o}C$. Therefore, an effective air circulation system surrounding the panel must be installed for heat exchanging to avoid unnecessary heating [34].In 1970 the second generation of solar cells appeared. Also known as the thin film solar cells, this group can be listed as amorphous silicon, Cadmium Telluride (CdTe) and Copper Indium Gallium di-Selenide (CIGS) cells. They are commercially found and applied extensively in utility-scale photovoltaic power stations, as they have better performance under cloudy conditions [37]. This thin film solar cell involves stacking up of very thin layers of the order of 1 µm of light absorbing materials on a substrates of plastic, glass or metals. Whereas the thickness of silicon wafers is 300 µm. Therefore, it may be appreciated that thickness of these cells is nearly 300 times thinner than the silicon wafers. In addition to lower thickness, these cells are comparatively flexible and attain lower weight than the conventional first generation cell [34].Nonetheless, the future environmental benefits and the potential scope of use of these solar cells may be limited by their elemental scarcity (In, Ga, Te) and toxicity (Cd). The term describing third generation solar cells is mostly used to describe systems which do not fall into the first or second generations, also known as multi-junction solar cells improved electrical conductivity while retaining very low manufacturing costs. Recent researches are aiming the efficiencies of 30–60% with low-priced materials and manufacturing techniques [34]. Types of various third generation cells are Organic solar cells (OSC), Quantum dots (QD) solar cells, Concentrated solar cells (CPV), Transparent solar cells (TSC), Perovskite solar cells (PSC). In order to better clarification the figure (II.7) summarize the classification of Solar Cells Technologies.

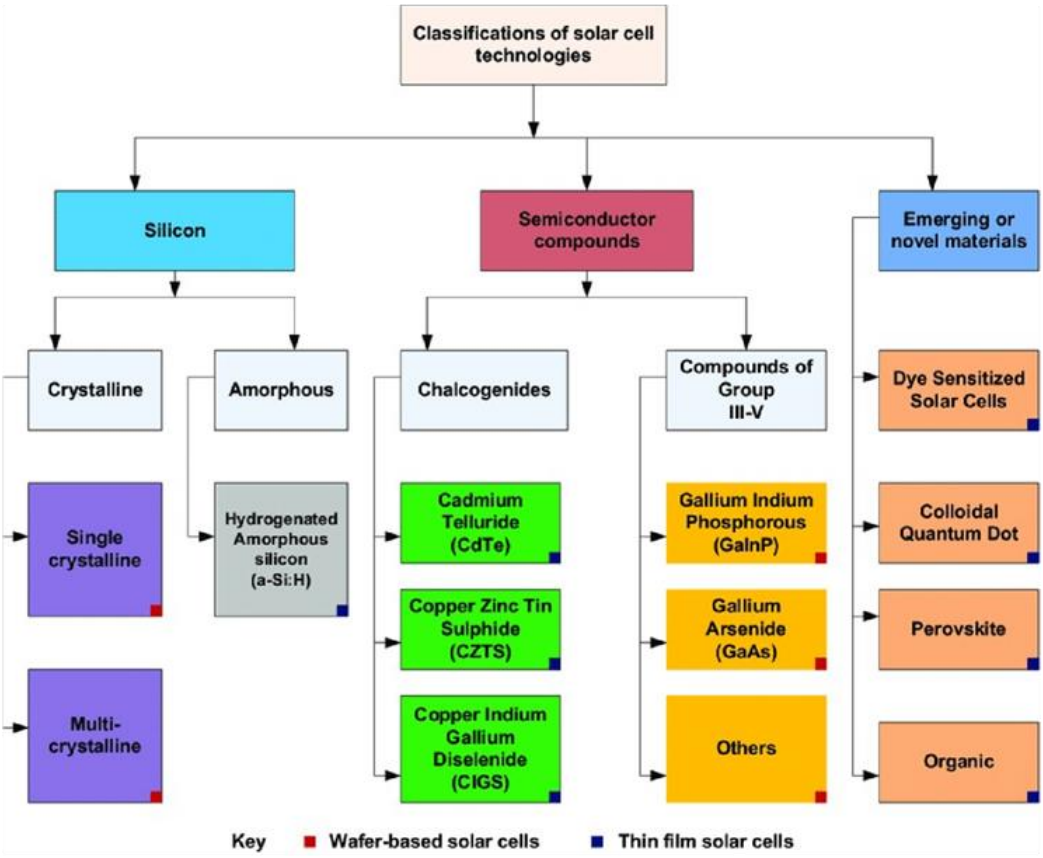


Fig.II.7. The classification of Solar Cells Technologies [38].

II.2.7. Thin films solar cells

A thin-film solar cell is a second generation solar cell that is made by depositing one or more thin layers or thin film of photovoltaic material on a substrate, such as glass, plastic or metal. Thin-film solar cells are commercially used in several technologies, including cadmium telluride (CdTe), copper indium gallium di-selenide (CIGS), and amorphous thin-film silicon (a-Si, TF-Si).

II.2.7.1 Amorphous Silicon Solar Cell (A-Si)

This type of solar cell was the most commonly known amongst thin films, though it has been on the market for over 15 years [39]. Amorphous-Si modules are produced by placing a tiny film of silicon vapor (approximately 1 µm thick) on a substrate material like glass or metal. A transparent conducting oxide (TCO) is incorporated in the set up to help reduce the series

resistance by providing a lateral conducting pathway for current [37].However, these cells can also perform satisfactorily at higher temperatures. Furthermore, these cells are adapted to variable weather conditions where intensity of sunlight is not optimum. The efficiency improvement of a-Si has seen a leap from 2.4% to 14 % between 1976 and 2020 [34].

II.2.7.2 Cadmium Telluride Solar Cell (CdTe)

Though Cadmium (Cd) is a highly toxic element and tellurium is available in scarcity yet Cadmium Telluride (CdTe) is a better selection for advancement of low cost photovoltaic device. Its manufacturing technology is inexpensive as well it provides the optimum band gap of approx. 1.45 eV which permits the absorption of light easily, resulting in increased efficiency of solar cell [34]. The efficiency improvement of CdTe cell has seen a jump from 6% to 22.1 % between 1972 [40] and 2020 [36].

II.2.7.3 Copper Indium Gallium Di-Selenide Solar Cell (CIGS)

Copper Indium Gallium Selenide (CIGS) is another kind of thin film solar cells where CIGS is used as absorber layer. The CIGS material is a solid solution of copper indium selenide (CIS) and copper gallium selenide. It has a chemical formula of $CuIn(1-x)Ga(x)Se_2$ .Where the value of x can vary from 0 (pure copper indium selenide) to 1 (pure copper gallium selenide) The bandgap of CIGS material varying continuously with x from about 1.0 eV (for copper indium selenide) to about 1.7 eV (for copper gallium selenide). [41] As CIGS material is used instead of CdTe as absorber layer, CIGS has advantage over CdTe in toxicity aspects. The efficiency improvement of CIGS cell has seen a jump from 4.5% to 23.3 % between 1976 [42] and 2020 [36].

Table II.2. Summary Highlights of Solar PV Technologies [37].

Solar Technology	Characteristics	Efficiency[36]	Advantages	Drawbacks
Monocrystalline	Made from pure monocrystalline silicon that has a single, continuous, crystal lattice structure with little or no impurities.	27.6%	1. Longevity 2. low installation cost 3. Non hazardous	1. High cost 2. Fragility 3. Silicon is wasted in the Czochralski process

Polycrystalline	Produced using numerous grains of monocrystalline silicon	23.3%	1. Simple production process 2. More heat tolerant than silicon based panels	1. Lower conversion efficiency than monocrystalline 2. Lower space efficiency
CIGS	Uses semiconductor layers of CIGS to absorb sunlight and convert to electricity	23.3 %	1. Uses little or no toxic material unlike CdTe 2. Have better resilience to heat than Si-based panels	1. Less efficient than monocrystalline panels
CdTe	Fabricated using a superstrate consisting of the successive layers of sodalime glass/ITO/CdS/CdTe/ back contact	22.1 %	1. Absorbs sunlight at shorter wavelength 2. Cost less to manufacture due to abundance of Cadmium material	1. Cadmium is very toxic 2. Disposal of old CdTe panels is a concern 3. Less efficient than C-Si
Amorphous Silicon	Composed of silicon atoms in a thin homogenous layer	14.01%	1. Multijunction device capacity 2. Easy fabrication 3. High optical absorption coefficient 4. Less toxic material than CIGS and CdTe 5. Flexible and less susceptible to cracks	1. Low efficiency

PSC	Utilizes ABX_3 crystal structure known as perovskite structure as an active light harvesting layer	25.7%	1. Cost effective fabrication 2. Cheap to scale up 3. Less space required for installation 4. High efficiency	1. Materials breakdown fast from exposure to heat, moisture, snow. 2. Material is toxic in nature

II.3. Conclusion

In this chapter we presented an overview on photovoltaic cells and their Principe of operation also the main parameters required to examine the capability of a solar cell as the short-circuit current density (J_{SC}), fill factor (FF), open-circuit voltage (V_{OC}) and power conversion efficiency. We also explained all the generations of solar cells and the advantages and disadvantages of each one of them, in addition to the recent conversion efficiency achieved. As described in this chapter, the current thin film technologies face some issues related to the cost (In, Ga), low abundance (In, Te), and environment (Cd). Therefore, current PV community has focused on the search for alternative absorber materials for future PV technologies, in this work alternative compound such as $CuSbS_2$, $CuSbSe_2$, $CuBiS_2$, and $CuBiSe_2$ have been suggested as PV absorber materials.

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CHAPTER III

Results and Discussion

III.1. Introduction

Given the many problems faced by the PV research community in realistic experiments researchers turned to simulations because of the high costs of the manufacturing technologies and the materials used in these experiments [1]. Numerical simulation has become necessary for all fields of research, especially in technological research, because simulation has become an important and necessary element of any work due to its advantages, and it allow us to study and design more easily. Simulation programs also allow us to save the work and modify it without having to start it over at the beginning. It also makes it possible to share it with other researchers**.**

Since the first generation, the photovoltaic cell industry has known some technical and economical obstacles. One of these difficulties represented in the chosen materials to manufacture these PV cells. The photovoltaic industry generations have shown a progression and variety in the last seventy years, starting with the crystalline silicon solar cells to the amorphous silicon (a-Si:H), Cadmium telluride (CdTe), Copper and indium selenide (CIS or CIGS), Organic cells , multi-junction and hybrid solar cells. The thin film solar cells technologies and materials have not achieved the desired efficiency in photovoltaic conversion in addition to their scarcity in nature and their cost. So, in our study we have focused on efficient and cheaper materials like $CuSbSe_2$ and $CuSbS_2$ [2]. In this work, by using the wxAMPS-1D package, we have studied and simulated a thin film solar cell based on $CuSbSe_2$ and $CuSbS_2$, the first is ZnO/CdS/$CuSbSe_2$ and the second is ZnO/CdS/$CuSbS_2$.

There are many photovoltaic simulators including: **wxAMPS-1D simulation software (**Analysis of Microelectronic and Photonic Structures-One Dimensional) [3.4], **SCAPS** (a Solar Cell Capacitance Simulator) [5], **ASA (**Advanced semiconductor analysis software**)** [6]**, PC 1D (**personal computer one dimensional**)** [7] and **SILVACO (**Silicon Valley Corporation) [8]. We have summarized some of the different characteristics of these simulators in the Table below (III.1).

Table III.1. Some simulators using in the study of thin film solar cells recently [9].

Characteristics	WxAMPS 1D	SCAPS	ASA	PC1D
Maximum number of layers	30	7	Unlimited	5
Discontinuities of the band in E_c and E_v	All programs use Anderson's model			
Gap gradual	No	No	Yes	No
profound state	50	3	4	No charge
Interface states	No	Yes	No	No
Changing in profound state	Yes	Yes	Yes	No
Digital robustness (convergence)	++	Ok	++	Ok
Fast	-	+	++	++
Easy to use	+	++	-	++

III.2. Presentation of the wxAMPS-1D simulator

Our chosen simulation software was the wxAMPS-1D (analysis of Microelectronic and Photonic Structures in one Dimension) which initially used for the analysis and design of transport phenomena in microelectronics and photonic structures [10]. The wxAMPS-1D was developed by the team of Professor Stephen Fonash in 1997 at the University of Pennsylvania in USA [11, 12] this software was developed in both UNIX and Windows versions. We preferred to use the most recent version (2012) on Windows 7 [11, 12]. This simulation tool provide to conduct any type of defect, gap energy and special distribution, also the incorporation of S-R-H recombination and band to band, integrate of Boltzmann and Fermi-Dirac statics, its ability to define the variable properties of materials, as well the contact

processing and the potential to handle transport in polarized devices, under illumination or both. It digitally solves the device's three equations (The **Poisson** equation, the continuity equation for free holes, and the continuity equation for free electrons) [13].

III.2.1.The wxAMPS-1D simulator functionality

III.2.1.1.Interface

The main user interface is described below (fig.III.1) allowing users to manipulate in the different function of the wxAMPS such us environmental conditions, materials properties, settings and showing results.

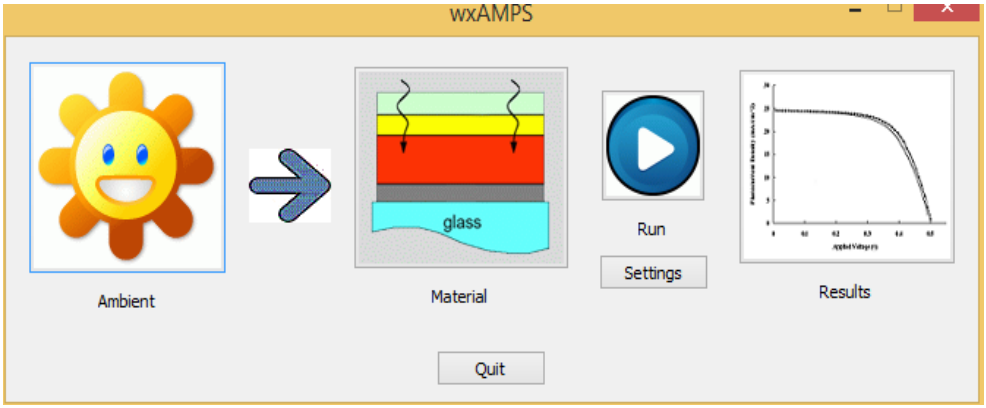

Fig.III.1. The home interface of wxAMPS-1D.

We can simulate with temperature and light at the intersection of environmental conditions. To investigate the effect of these parameters on the performance of the PV cell, the temperature was set to 300 °K (ambient temperature) with the option of darkness or lighting. This wxAMPS-1D interface is shown in Figure (III.2).

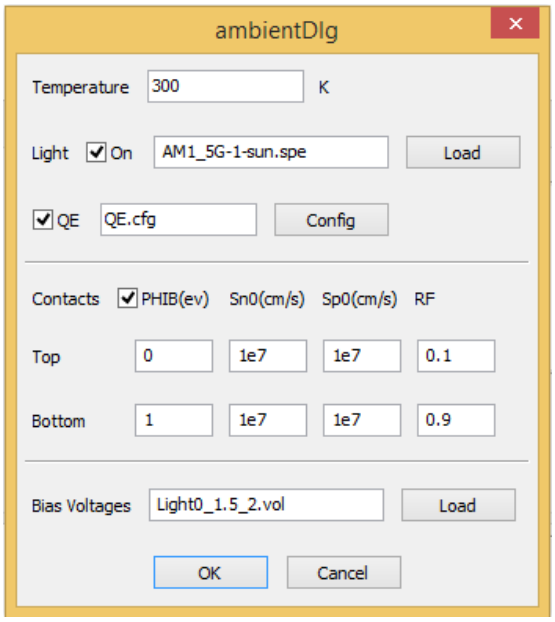

Fig. III.2. The environmental conditions window.

The physical parameters of the material for each layer of the proposed structures must be fixed. For regular simulation of ZnO/CdS/$CuSbSe_2$ and ZnO/CdS/$CuSbS_2$ the layer's material thickness, electrical properties (gap energy, mobility, affinity, doping...), optical qualities, and flaws are all mentioned. Through alterations to the material properties interface, it is possible to determine the effect of thickness and doping for each layer on the characteristics of the cell to achieve maximum performance.

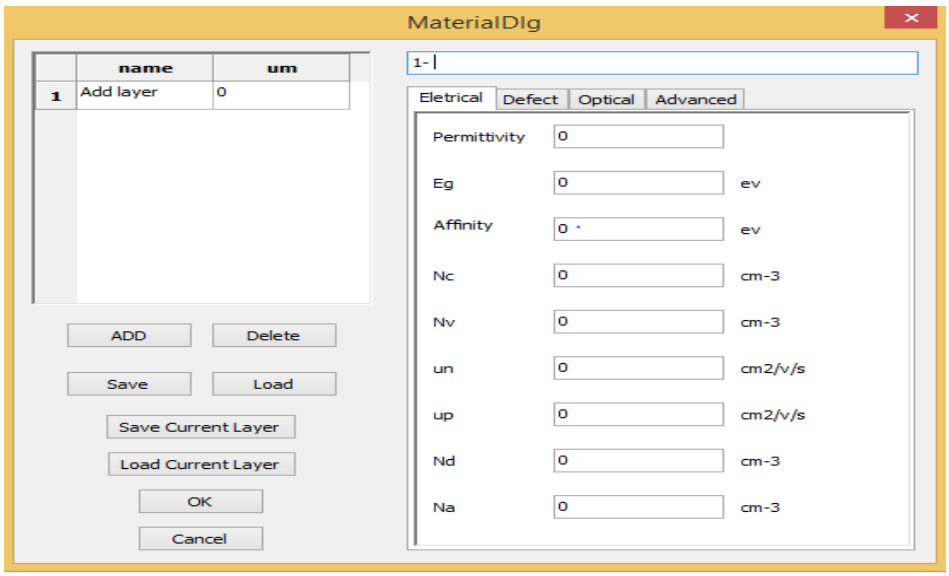

Fig.III.3. The interface of the material properties of each layer.

When the calculation is complete, the results are stored and presented by curves. They are the characteristics (J-V) in the dark and under illumination, the values of the saturation current density (J_0), the factor ideality (A), parallel resistance (shunt) R_{sh}, resistance series R_s , density short circuit current (J_{cc}), open circuit voltage (V_{oc}), filling (FF), photovoltaic conversion efficiency, quantum efficiency external (EQ) as well as internal quantities such as the energy gap diagram, densities of free or trapped carriers, field and electric potential, rate of recombination, the components of the current of electrons and holes, the durations of life... etc. The tape-to-tape model currently requires a lot of time to achieve a solution (~30 minutes for an I-V curve of a 2000 grid device), and sometimes it may fail during convergence. In order to increase the convergence property, the following methods can be tried [14]:

- Adjust the grids. Especially for the tunnel junction, a well-refined grid is highly recommended.
- Adjust the numeric setting, such as increasing the time limit iteration (> 5000), convergence accuracy setting (1e-8~1e-9) and set with "Clamping Range".
- Reduce voltage steps if the simulation fails at high voltage.

III.3. Material parameters and device structure

In this study, the performance of the device structure with three different layers is optimized, ZnO has taken as the window layer, CdS as a buffer layer, $CuSbS_2$ or $CuSbSe_2$ adopted as an absorber layer. Mo has been taken as a back Contact and AZO layer serves as front contact. The device structure of our studied photovoltaic cell is illustrated in Figure (III.4).

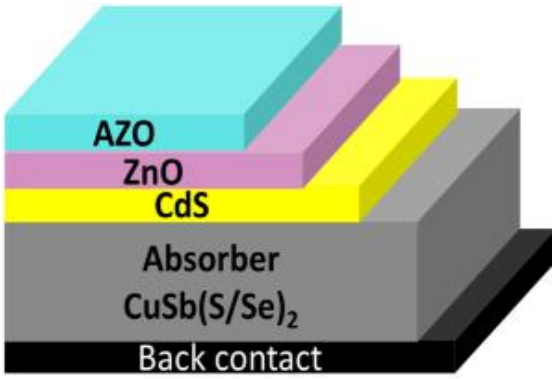

Fig.III.4. Device structure of the solar photovoltaic cell [2].

The parameters of the different layers constituting the structure of the Figure (III.4) are shown in Table (III.2).

Table.III.2. The material's parameters of different layers.

Material Properties	**$CuSbS_2$**[2]	**$CuSbSe_2$**[2]	**CdS** [15]	**ZnO**[15]
Thickness[um]	2.5	2.5	0.01	0.01
Permittivity	10	10	10	9
Eg [ev]	1.45	1.08	2.4	3.4
Affinity [ev]	4.05	4.11	4.0	4.35
Nc [cm-3]	$1.23x10^{20}$	$9.9x10^{19}$	$2.2x10^{18}$	$2.2\,x10^{18}$
Nv [cm-3]	$1.78x10^{20}$	$9.9x10^{19}$	$1.8x10^{19}$	$1.8x10^{19}$
Un [cm2/Vs]	4	10	100	100
Up [cm2/Vs]	4	10	25	25
Nd [cm-3]	0	0	$1x10^{18}$	$1x10^{18}$
Na [cm-3]	$1x10^{20}$	$1x10^{20}$	0	0

III.4. Simulation and results

III.4.1. The first proposed solar cell

In this part of our work, we have studied the first proposed structure (ZnO/CdS/$CuSbSe_2$) (figure III.4).based on the physical parameters obtained from Table (III.2).To obtain the best simulation results, we have optimized the layers thicknesses and doping concentrations.

III.4.1.1. Layer's thicknesses optimization

III.4.1.1.1. Effect of ZnO layer thickness

Table.III.3. Photovoltaic parameters for different thicknesses values of the ZnO layer.

ZnO thickness (um)	V_{oc} (v)	J_{sc} (mA/cm^2)	FF (%)	η (%)
0.01	0.4672	27.6908	78.4003	10.1429
0.02	0.4672	27.7124	78.3067	10.1390
0.03	0.4672	27.6950	78.3017	10.1316
0.04	0.4672	27.6830	78.3032	10.1271
0.05	0.4672	27.6684	78.3001	10.1211
0.06	0.4672	27.6563	78.3006	10.1164
0.07	0.4671	27.6427	78.2983	10.1108
0.08	0.4671	27.6294	78.2964	10.1055
0.09	0.4671	27.6175	78.2964	10.1008
0.1	0.4671	27.6046	78.2947	10.0956

Figure (III.5) and (III.6) represents the efficiency and fill factor values in terms of the thickness of ZnO layer.

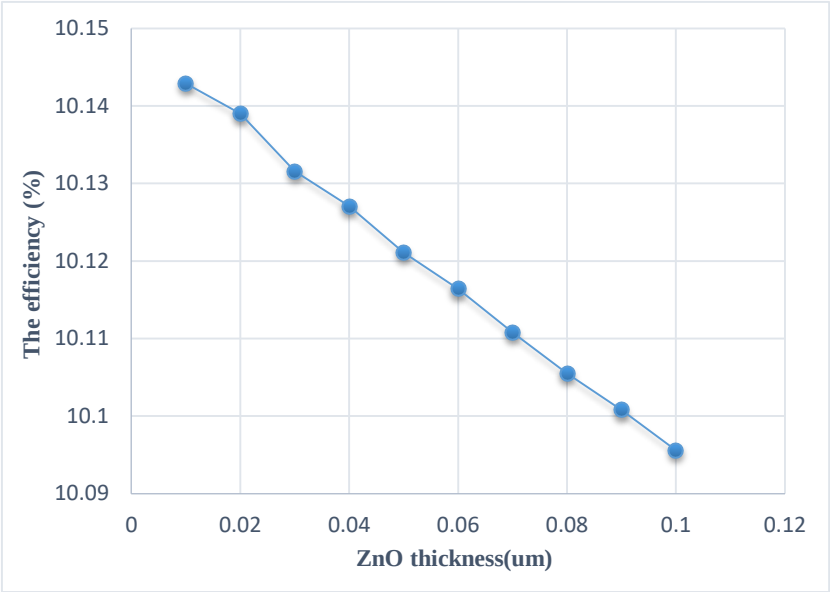

Fig.III.5. Variation in the efficiency as a function of the thickness of the ZnO layer.

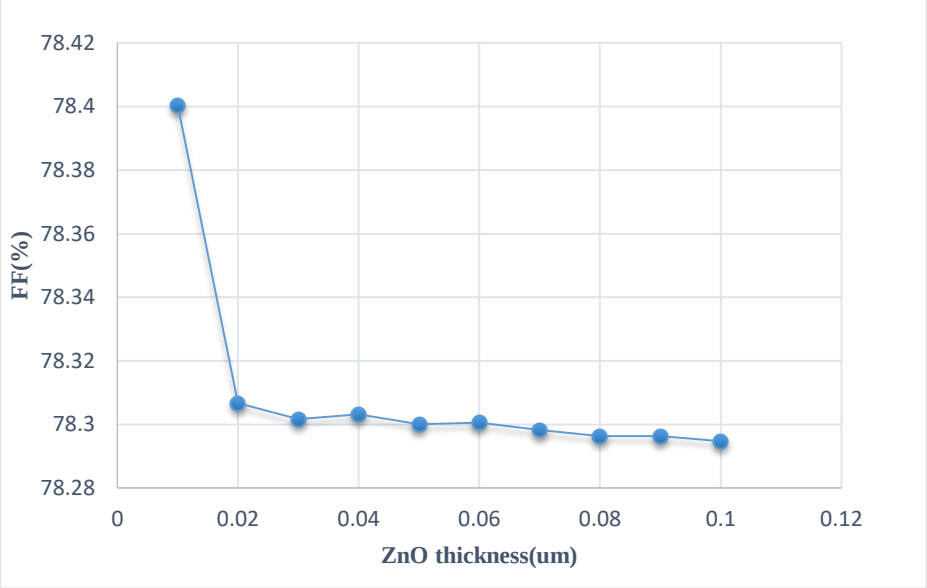

Fig.III.6. Fill factor variation as a function of ZnO layer thickness.

From optimizing the window layer (ZnO layer) it is found that the more we increase the thickness of the layer the more the efficiency is decreased, and for best performance the thickness of the window layer must be thin, and using a material with a large band gap to avoid front surface recombination.

III.4.1.1.2. Effect of CdS layer thickness

Table.III.4. Photovoltaic parameters for different thicknesses values of the CdS layer.

CdS Thickness (um)	V_{oc} (v)	J_{sc} (mA/cm^2)	FF (%)	η (%)
0.01	0.4672	27.6908	78.4003	10.1429
0.02	0.4643	24.8693	78.3144	9.0438
0.03	0.4638	24.3067	78.2447	8.8202
0.04	0.4633	23.9024	78.1821	8.6586
0.05	0.4629	23.4514	78.1074	8.4785
0.06	0.4625	23.1010	78.0445	8.3385
0.07	0.4621	22.7350	77.9752	8.1923
0.08	0.4618	22.4068	77.9092	8.0612
0.09	0.4615	22.1354	77.8514	7.9528
0.1	0.4612	21.8610	77.7905	7.8431

Figure III.7 and III.8 represents the conversion efficiency and fill factor values in terms of the thickness of the buffer layer CdS.

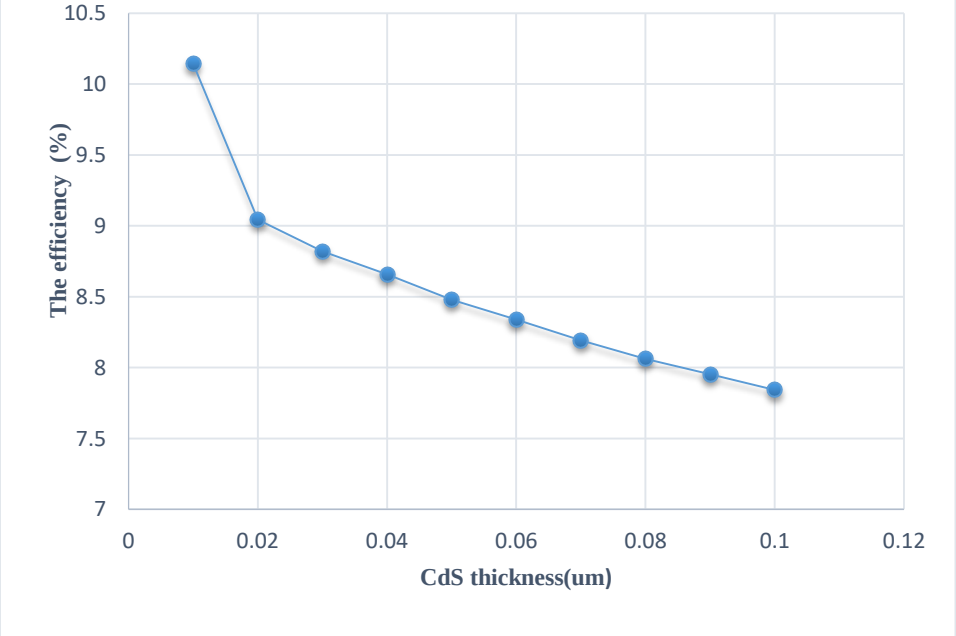

Fig.III.7. Variation in the efficiency as a function of the thickness of the CdS layer.

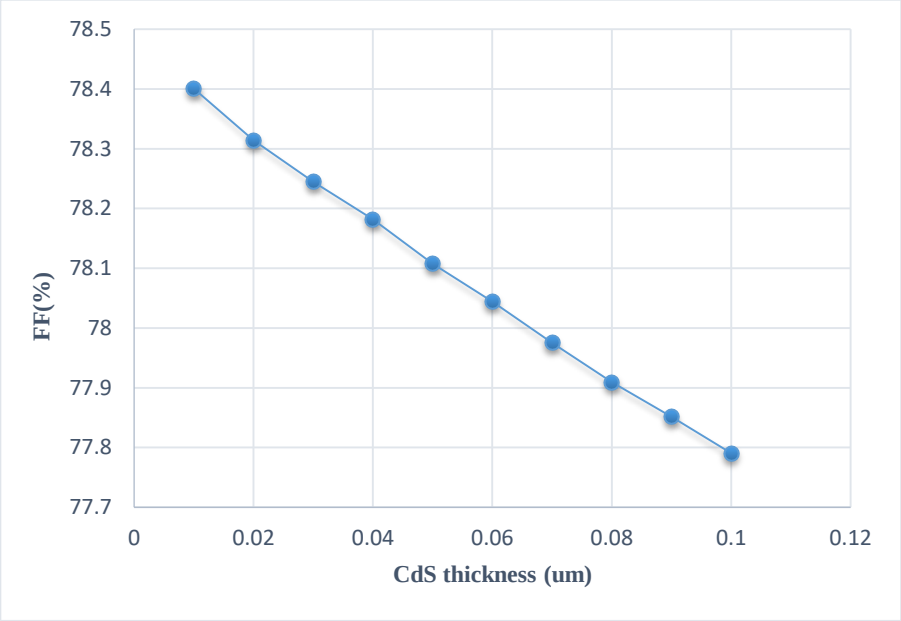

Fig.III.8. Fill factor variation as a function of CdS layer thickness.

A wide band gap material for the buffer layer is an obvious choice as it remains transparent to the lower energy photons and allows the maximum photon to pass through it to the absorber layer. The cadmium sulfide "CdS" acts as a material of choice for n-type heterostructure for P-type chalcogenide absorber solar cells [2]. The impact of CdS layer thickness on $CuSbSe_2$ device performance is computed and summarized in Table (III.4).We noticed that J_{sc} decreases, while V_{oc} remains nearly constant with increasing CdS layer thickness.

III.4.1.1.3. Effect of $CuSbSe_2$ layer thickness

Table.III.5. Photovoltaic parameters for different thicknesses values of the $CuSbSe_2$ layer.

$CuSbSe_2$ thickness (um)	V_{oc} (v)	J_{sc} (mA/cm^2)	FF (%)	η (%)
0.5	0.4673	27.7238	78.4249	10.1599
1	0.4672	27.6986	78.4163	10.1472
1.5	0.4672	27.6937	78.4109	10.1449
2	0.4672	27.6918	78.4056	10.1437
2.5	0.4672	27.6908	78.4003	10.1429
3	0.4672	27.6903	78.3951	10.1423

Figure (III.9) and (III.10) represents the efficiency and fill factor values in terms of the thickness of the absorber layer $CuSbSe_2$.

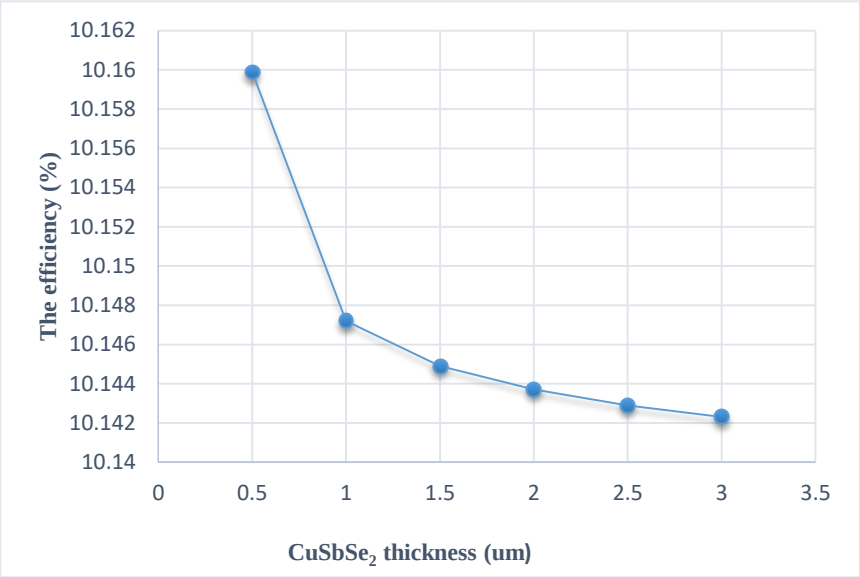

Fig.III.9. Variation in the efficiency as a function of the thickness of the $CuSbSe_2$ layer.

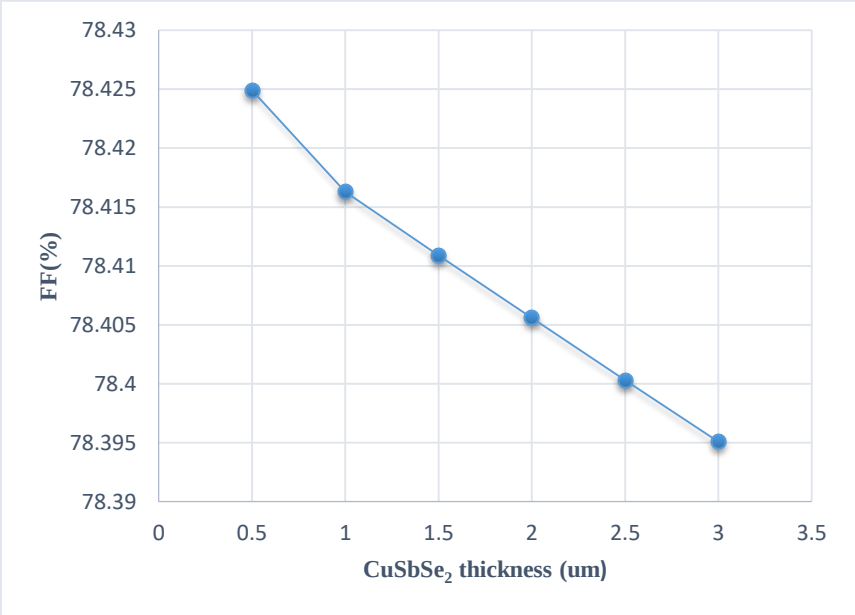

Fig.III.10. Fill factor variation as a function of $CuSbSe_2$ layer thickness.

After performing simulations using different values of the absorber layer thickness the results are summarized in Table (III.5), we notice that the results remain almost constant, but with slight difference we choose 0.5um as the optimal thickness value for the $CuSbSe_2$ layer.

III.4.1.1.4. The optimal thickness values for each layer

Table.III.6. the optimal thickness values of the structure ZnO_CdS_$CuSbSe_2$.

$CuSbSe_2$ (um)	CdS (um)	ZnO (um)
0.5	0.01	0.01

III.4.1.1.5. The performance of the cell for optimal thickness values

The optimized thicknesses values of the layers give us the photovoltaic parameters summarized in Table (III.7).

Table.III.7. The PV parameters obtained from the simulation.

J_{sc} (mA/cm^2)	V_{oc} (v)	η (%)	FF (%)
27.7238	0.4672	10.1599	78.4249

III.4.1.2. Layer's doping optimization

Using the optimal thickness values of the structure (ZnO/CdS/$CuSbSe_2$) obtained from the simulation (Table.III.6), the effect of cell performance of $CuSbSe_2$ doping concentration within the range 10^{15} -10^{20} is analyzed as shown in Table (III.8).

Table.III.8. Photovoltaic parameters for different doping values of the $CuSbSe_2$ layer.

Doping (cm^{-3})	V_{oc} (v)	J_{sc} (mA/cm^2)	FF (%)	η (%)
10^{15}	0.4589	27.8267	71.8454	9.1735
10^{16}	0.4510	27.8229	73.6707	9.2438
10^{17}	0.4865	27.5992	77.6412	10.4246
10^{18}	0.5481	26.5808	77.5872	11.3028
10^{19}	0.6051	25.3681	81.4817	12.5078
10^{20}	0.6612	25.2942	84.8528	14.1921

III.4.1.2.1. The optimal doping value and the performance of the cell

We have lunched the simulation with 10^{20} cm^{-3} as the ideal doping concentration. The obtained photovoltaic parameters are shown in Table (III.9).

Table.III.9. The PV parameters achieved after applying the optimal doping value.

$CuSbSe_2$ doping (cm^{-3})	**V_{oc} (v)**	**J_{sc} (mA/cm^2)**	**FF (%)**	**η (%)**
10^{20}	0.6612	25.2942	84.8528	14.1921

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- The current-voltage (J-V) characteristic of the first solar cell is shown in the figure.III.11.

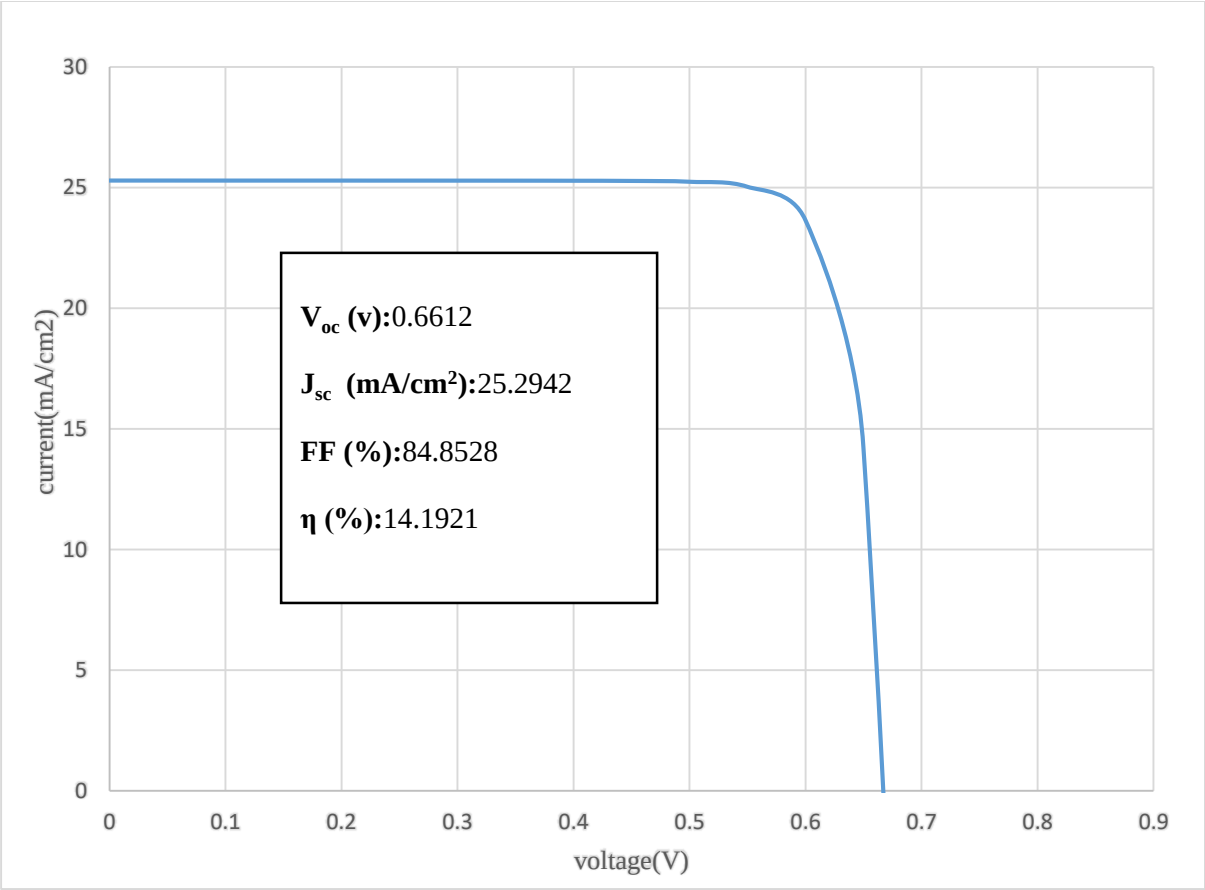

Fig.III.11. The current-voltage (J-V) characteristic of the $CuSbSe_2$ solar cell.

III.4.2. The second proposed solar cell

We have studied the second proposed solar cell with the structure ($ZnO/CdS/CuSbS_2$)(fig.III.13) according to the physical parameters in Table (III.2).For best results we optimized the layers thicknesses and the doping concentration.

III.4.2.1. Layer's thickness optimization

III.4.2.1.1. Effect of ZnO layer thickness

Table.III.10. Photovoltaic parameters for different thicknesses values of the ZnO layer.

ZnO thickness (um)	V_{oc} (v)	J_{sc} (mA/cm^2)	FF (%)	η (%)
0.01	0.8246	25.7438	79.3256	16.8394
0.02	0.8242	25.7293	78.9117	16.7346
0.03	0. 8242	25.7118	78.8990	16.7198
0.04	0. 8242	25.7011	78.9074	16.7145
0.05	0. 8242	25.6868	78.9005	16.7032
0.06	0. 8241	25.6757	78.9050	16.6967
0.07	0. 8241	25.6624	78.9004	16.6867
0.08	0. 8241	25.6497	78.8972	16.6773
0.09	0. 8241	25.6385	78.8999	16.6704
0.1	0. 8241	25.6262	78.8973	16.6613

Figure (III.12) and (III.13) Represents the conversion efficiency and fill factor values in terms of the thickness of ZnO layer.

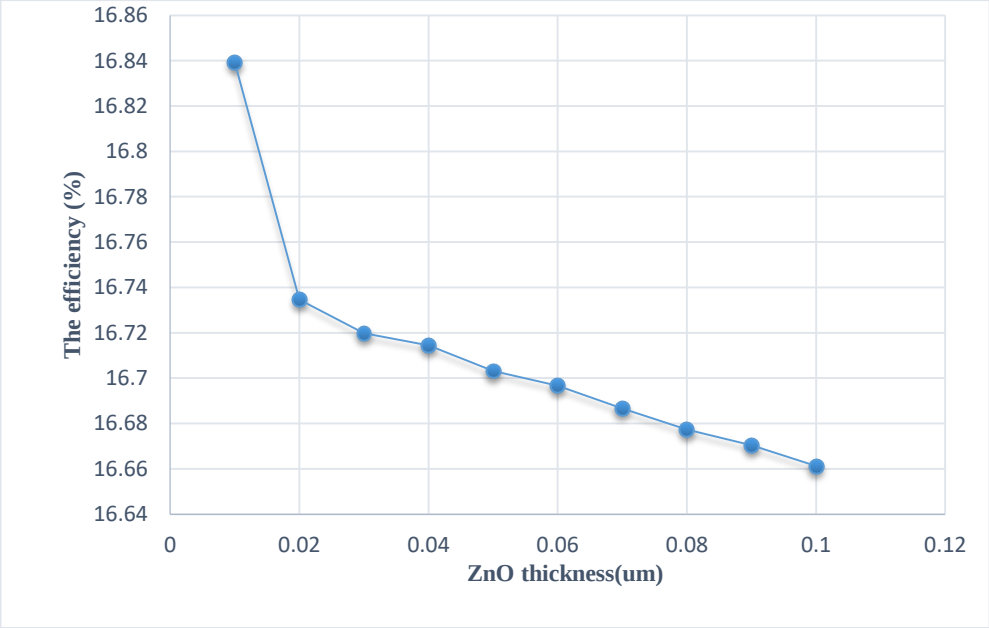

Fig.III.12. Variation in the efficiency as a function of the thickness of the ZnO layer.

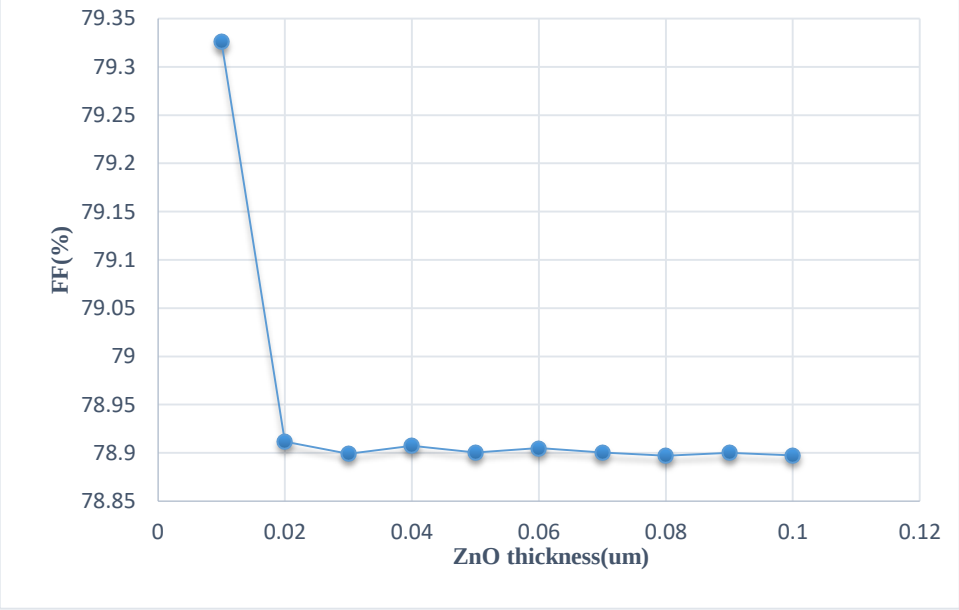

Fig.III.13. Fill factor variation as a function of ZnO layer thickness.

By optimizing the ZnO layer it is found that increasing the thickness of the layer has a negative effect on the efficiency, and for a window layer for the second solar cell we have found 0.01um as an ideal thickness value.

III.4.2.1.2. Effect of CdS layer thickness

Table.III.11. Photovoltaic parameters for different thicknesses values of the CdS layer.

CdS Thickness (um)	V_{oc} (v)	J_{sc} (mA/cm^2)	FF (%)	η (%)
0.01	0.8246	25.7438	79.3256	16.8394
0.02	0.8220	23.7013	80.0236	15.5912
0.03	0.8213	23.1740	80.0125	15.2278
0.04	0.8206	22.7588	79.9855	14.9385
0.05	0.8200	22.3240	79.9560	14.6361
0.06	0.8194	21.9683	79.9275	14.3882
0.07	0.8189	21.6127	79.8981	14.1408
0.08	0.8184	21.2919	79.8693	13.9176
0.09	0.8180	21.0173	79.8418	13.7263
0.1	0.8176	20.7488	79.8142	13.5394

Figure (III.14) and (III.15) represents the conversion efficiency and fill factor values in terms of the thickness of the buffer layer CdS.

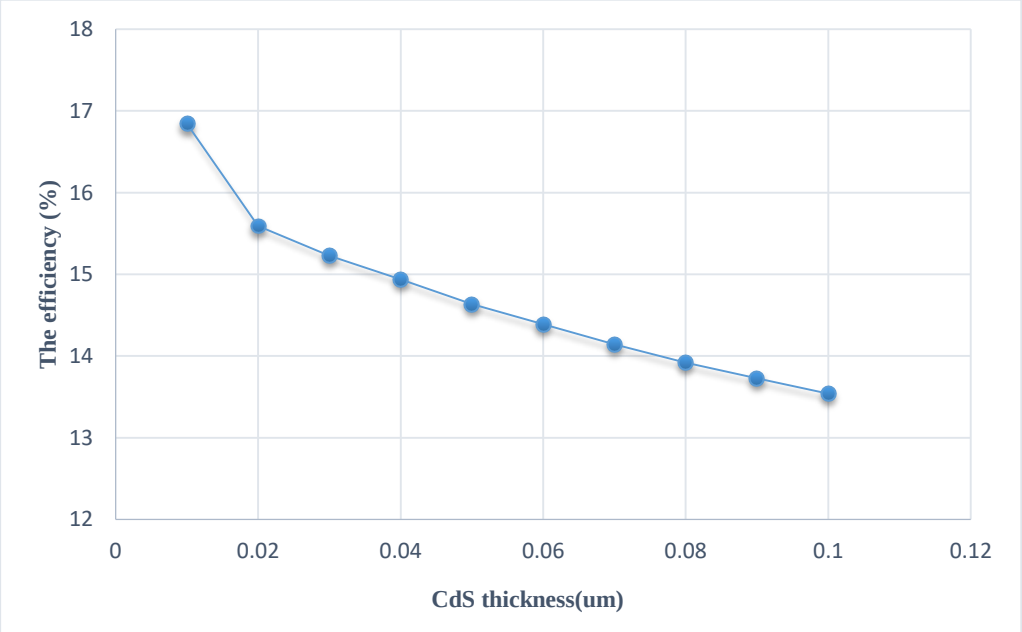

Fig.III.14. the variation in the efficiency as a function of the thickness of the CdS layer.

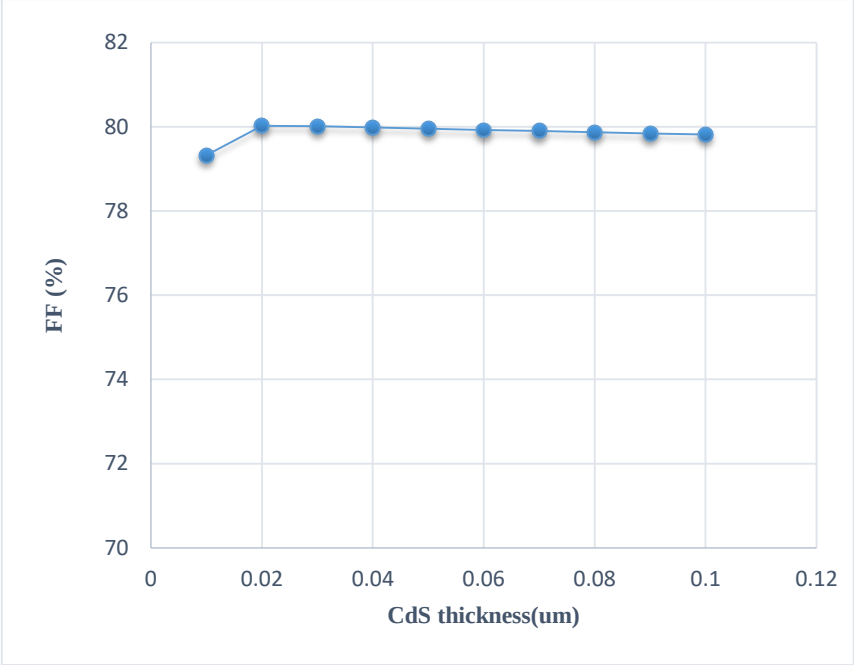

Fig.III.15. Fill factor variation as a function of CdS layer thickness.

The effect of the buffer layer thickness on the second solar cell performance is computed and summarized in Table (III.11), we observe that by increasing the thickness of the CdS layer the short circuit voltage and current density is decreasing and as well as the efficiency.

III.4.2.1.3. Effect of $CuSbS_2$ layer thickness

Table.III.12. Photovoltaic parameters for different thicknesses values of the $CuSbS_2$ layer.

$CuSbS_2$ thickness (um)	V_{oc} (v)	J_{sc} (mA/cm^2)	FF (%)	η (%)
0.5	0.8331	25.7175	79.4615	16.8198
1	0.8245	25.7509	79.3378	16.8450
1.5	0.8246	25.7464	79.3321	16.8419
2	0.8246	25.7446	79.3289	16.8403
2.5	0.8246	25.7438	79.3256	16.8394

Figure (III.16) and (III.17) represents the conversion efficiency and fill factor values in terms of the thickness of the absorber layer $CuSbS_2$.

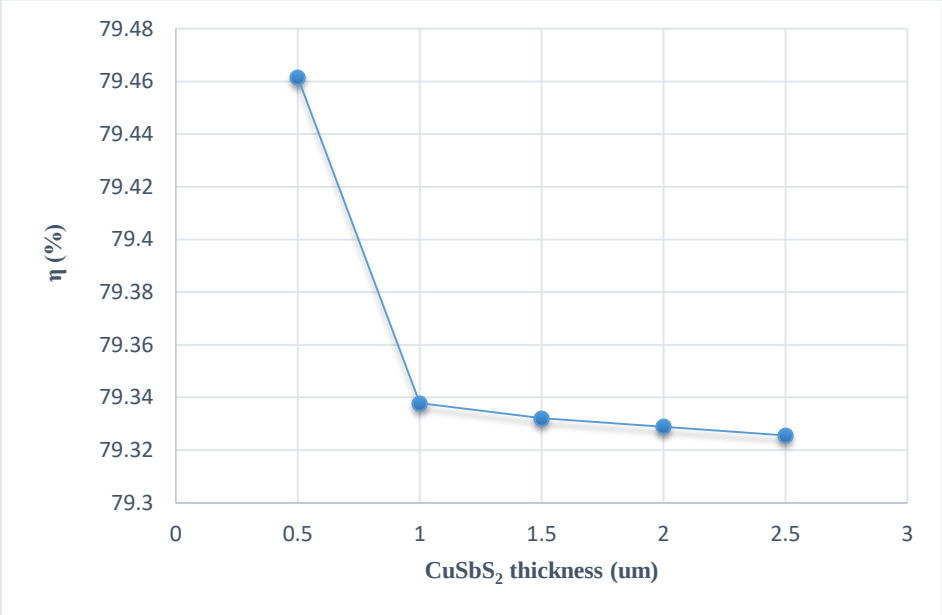

Fig.III.16. Variation in the efficiency as a function of the thickness of the $CuSbS_2$ layer.

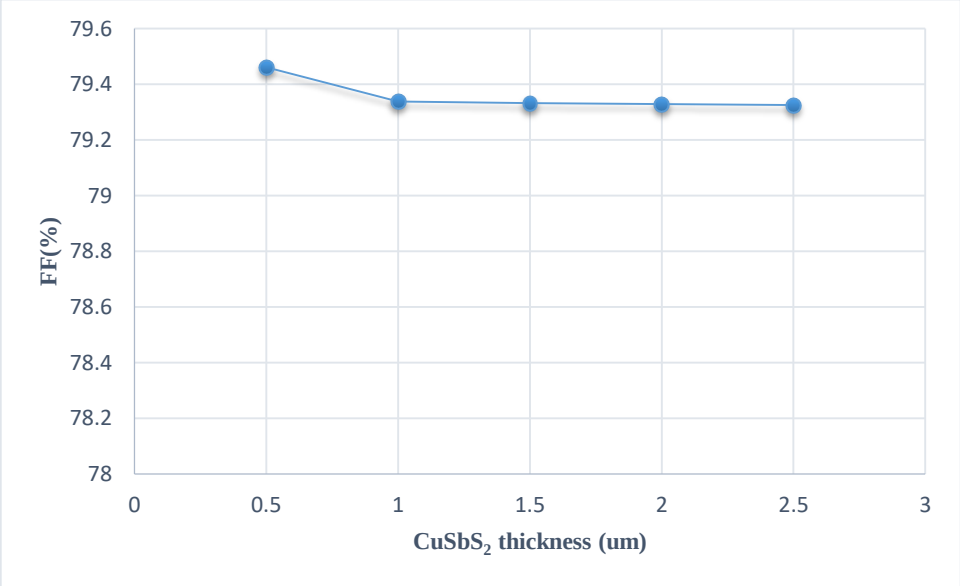

Fig.III.17. Fill factor variation as a function of $CuSbS_2$ layer thickness.

After simulations for different absorber thickness values, the PV parameters for each simulation are shown in Table (III.12).the V_{oc} almost remain the same but we notice a decrease in the J_{sc} and the efficiency by increasing the thickness of the $CuSbS_2$ layer.

III.4.2.1.4. The optimal thickness values for each layer

Table.III.13. The optimal thickness values of the structure ZnO_CdS_$CuSbS_2$.

$CuSbS_2$ (um)	CdS (um)	ZnO (um)
1	0.01	0.01

III.4.2.1.5. The performance of the cell for optimal thickness values

The optimized thicknesses values of the layers give us the photovoltaic parameters summarized in Table (III.14).

Table.III.14. the PV parameters obtained from the simulation.

J_{sc} (mA/cm^2)	V_{oc} (v)	FF(%)	η (%)
0.8245	25.7509	79.3378	16.8450

III.4.2.2. Layer's doping optimization

Based on the optimal thickness values for each layer of the structure (ZnO/CdS/$CuSbS_2$) (summarized in Table (III.13)), we studied the effect of the doping concentration on the performance of the second solar cell.

Table.III.15. Photovoltaic parameters for different doping values of the $CuSbS_2$ layer**.**

Doping (cm^{-3})	V_{oc} (v)	J_{sc} (mA/cm^2)	FF (%)	η (%)
10^{15}	0.7326	26.9161	78.8809	15.5548
10^{16}	0.8014	26.5856	78.5869	16.7440
10^{17}	0.8450	25.2317	79.5267	16.9554
10^{18}	0.9016	22.9489	80.8748	16.7344
10^{19}	0.9590	21.0512	87.0921	17.5820
10^{20}	1.0169	20.8709	88.7702	18.8405

III.4.2.2.1. The optimal doping value and the performance of the solar cell

After starting the simulation and choosing the optimal doping concentration for this cell (10^{20} cm^{-3}) the PV parameters obtained are shown in Table III.16.

Table.III.16. The PV parameters achieved after applying the optimal doping value.

$CuSbS_2$ doping (cm^{-3})	V_{oc} (v)	J_{sc} (mA/cm^2)	FF (%)	η (%)
10^{20}	1.0169	20.8709	88.7702	18.8405

- The current-voltage (J-V) characteristic of the $CuSbS_2$ solar cell is shown in the figure.III.18.

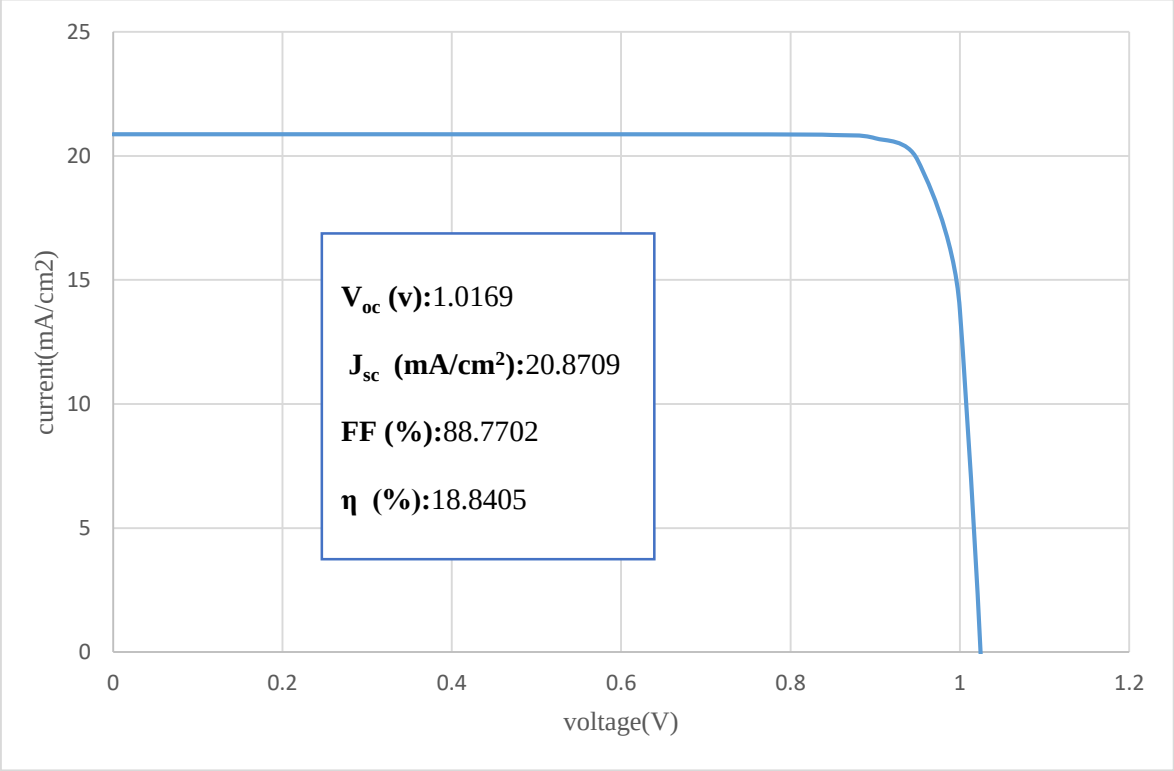

Fig.III.18. The current-voltage (J-V) characteristic of the $CuSbS_2$ solar cell.

In Table (III.17), we have summarized the PV parameters of the obtained results with the perovskite, CIGS, CZTS, CdTe solar cells.

Table.III.17. A review on Different thin film solar cells with our results.

PV parameters	perovskite[9]	CIGS[9]	CZTS[15]	CdTe[16]	$CuSbSe_2$	$CuSbS_2$
V_{oc} [V]	1.03	0.72	0.89	0.859	0.6612	1.0169
J_{sc} [mA/cm^2]	22.65	38.42	18.619	28.4	25.2942	20.8709
FF [%]	80.20	84.88	77.6	73.7	84.8528	88.7702
η [%]	18.75	23.49	12.92	17.66	14.1921	18.8405

III.5. Conclusion

In this chapter, have been performed a simulation for $CuSbSe_2$ and $CuSbS_2$ based thin-film solar cells using wxAMPS package. The efficiency of the solar cells has been optimized by varying the thickness and doping concentrations of TCO layers, buffer layers, and absorber layers. Moreover, the obtained maximum efficiencies are approximately 14.19 % and approximately 18.84 %, for $CuSbSe_2$ and $CuSbS_2$ based solar cell, respectively. Thus, it is hoped that this study will help the PV community (scientists, researchers and manufacturers) to understand the behavior of $CuSbse_2$ and $CuSbS_2$ thin film solar cells and to fabricate non-toxic, earth-abundant less-complex and high-efficiency thin film solar cells in the near future. As perspective, these results encourage us to lunch a similar investigations on $CuBi(SSe)_2$ based solar cells.

III.6. References

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General conclusion

This work is focused on the study by numerical simulation of the thin film solar cells based on chalcostibites materials, with the aim of designing an optimal structure, giving the best possible electrical efficiency. The simulation numerical analysis was carried out using (analysis of Microelectronic and Photonic Structures in one Dimension) AMPS - 1D simulator.

Therefore, a bibliographical study was carried out, in order to allow us to better understand the subject of our study. At first, we introduced the chalcostibites materials and the proposed compounds for our study by presenting their crystal structure and their optical and electrical properties.

Then we previewed the basic concepts of PV solar cells and their types, as well as the generations that have passed through the manufacture of solar cells, In addition to the advantages and disadvantages of each type.

Also a part of this work was devoted to the relatively detailed presentation on the AMPS-1D simulation software and the proposed structures with the physical parameters of each one.

Finally, we have presented and treated our results from the numerical simulation of the studied structure, within the wxAMPS-1D. We have started by modelling and simulating the first proposed solar cells with the structure (ZnO /CdS/$CuSbSe_2$), The efficiency of the solar cell have been observed by varying the thickness and the doping concentrations of TCO layer (ZnO) , buffer layers(CdS) , and the absorber layer ($CuSbSe_2$). Moreover, from the simulation, the maximum efficiency has been achieved by 14.19 %. And by repeating the same steps with the second proposed solar cell with the structure (ZnO/CdS/$CuSbS_2$), we find that the efficiency reaches 18.84%.

The two studied solar cells show promising results, and both $CuSbS_2$ and $CuSbSe_2$ thin film absorbers display the desired optical and characteristics for PV applications, but further analysis is required for their integration in efficient devices, and it is hoped that this study will help the students, scientists, researchers and manufacturers to understand the behaviour of $CuSb(SSe)_2$ thin film solar cells and to fabricate high-efficiency thin film solar cells in the near future. As perspective, these results encourage us to lunch a similar investigations on $CuBi(SSe)_2$ based solar cells.