N° d'ordre :


**UNIVERSITE KASDI MERBAH OUARGLA**

FACULTE DES MATHEMATHIQUES

ET DES SCIENCES DE LA MATIERE

**DEPARTEMENT DE PHYSIQUE**


# Mémoire

**MASTER ACADEMIQUE**

Domaine : Sciences de la Matière

Filière : Physique

Spécialité : Physique énergétique et énergie renouvelable


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**Thème :**

# Simulation of thin film solar cells using the SCAPS-1D program

Soutenu publiquement

Le : 18 / 06 / 2023

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Année Universitaire: 2022/2023

# Acknowledgements

First and foremost, I would like to thank **God** Almighty for giving me the strength, knowledge, ability and opportunity to undertake this research study and to persevere and complete it satisfactorily. Without his blessings, this achievement would not have been possible.

I would like to thank the following people for helping with this research project:

I express my gratitude to **Pr. Babahani Oum-El-Kheir** as supervisor of this work, by her knowledge, time, dedication, guidance, support, encouragement and invaluable advices throughout of this work to achieve the Master degree.

Furthermore, I would like to express my sincere thanks to the members of jury: **Dr. BEN BELGACEM Khalfallah** as a president of jury, and **Dr. LEMKEDDEM Soumaya** as examiner for their acceptance to evaluate and examine my work.

My sincer gratitude to all those who have helped me near or far to do this work.

# Dedication

I dedicate this modest work to:

**My dear parents**

For all their sacrifices, their love, their tenderness, their support

and their prayers Throughout my studies

For all my **siblings**

And of course to **my family**

To all **my friends**

**Hala KHELFAOUI**

# Summary

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# Abbreviations list

| | |
|---|---|
| **AC** | Alternating Current |
| **CB** | Effective Density of States |
| **CV** | Effective Density of States |
| **CVD** | Chemical Vapor Deposition |
| **DC** | Direct Current |
| **ETA, ŋ** | Efficinecy |
| $E_g$ | Energy Band |
| $E_v$ | Valence Band |
| $E_c$ | Conduction Band |
| **FF** | Fill Factor |
| $I_{max}$ | Maximum current |
| $I_{ph}$ | Photon Current |
| $I_{sc}$ | Shor Circuit Current |
| **ITO** | Indium Tin Oxide |
| $N_A$ | Acceptor Density |
| $N_c$ | Conduction Band Density |
| $N_D$ | Donor Density |
| $N_v$ | Valence Band Density |
| **OPV** | Organic Photovoltaic |
| **PV** | Photovoltaic |
| $P_{max}$ | Maximum Power Point |
| $R_s$ | Series Resistance |
| $R_{sh}$ | Shunt Resistance |
| $V_{oc}$ | Open Circuit Voltage |
| $V_{max}$ | Maximum Voltage |
| $V_{th}$ | Thermodynamics Voltage |

# General introduction

# General introduction

Many countries rely on the use of fossil energies such as gas and oil. These energies, in addition to being unclean, are not renewable. Due to the increasing demand for energy, environmental organizations encourage the use of alternative energy sources such as solar energy. Solar energy is the most affordable, abundant, renewable and clean of all long-term natural resources to date [1]. Solar PV (photovoltaic) systems are a renewable energy technology that allows the utilization of solar energy directly from the sun to meet electricity demands [2]. Solar cells are being developed year by year and become more easy to use and have different applications. To keep up with times, solar cells are is tend to rely on nanotechnology. Thin film or nano solar cells, like other solar cells, are built of electronic semiconductors that use the photoelectric effect. It have several applications most notably the production and the storage of energy and manufacture of smart materials in communications[3]. And because of the difficulty of conducting experiments on thin film solar cells, scientists went to simulate these cells and then manufacture them after obtaining results with interesting specifications of purity, accuracy and thickness in order to make the best use of them. Simulation is an essential tool for optimizing the structure and the different parameters of solar cells and usually requires an effective system such as SCAPS-1D program. This program is being used in various studies due to its most accessible and straightforward method and also allows the simulation of solar cells from one to seven layers.

In this work, we are going to test the performance parameters of thin film Solar cells which will be analyzed by studying the characteristics of the layers using numerical simulation with SCAPS-1D program.

Variations in layer thickness, temperature, series and shunt resistance and absorber and ITO layers will be used to investigate the properties of solar cell. The fill factor (FF) and efficiency of the layers will be determined and examined in each of these examples.

This Thesis is organized as follows: After a general introduction

1. The **first chapter**, where we will introduce firstly solar energy, semiconductors, doping, solar cells and its different structure and we will focus on thin films solar cells, namely the working principle and electrical characterizations.
2. The **second chapter** we will explore and demonstrate SCAPS-1D program, its different materials and the way you can use this program to obtain numerical results.

3. In the **third chapter,** we will study the effect of temperature, thickness, series and shunt resistance, absorber layer and ITO layer on solar cell characteristics., we will compare between SCAPS-1D and AFORS-HET results. And we will compare between two solar cells simulated with SCAPS-1D.

Finally , we will end this thesis with a conclusion that resume our work and the main results we will obtain from simulation.

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# Chapter 01 : Generalities about solar cells

## Introduction

In this chapter, we talk about general information about solar cells. Starting with definitions of solar energy, solar radiation, semiconductors, and doping. Next, we will talk about solar cells and their types. Finally, we will focus on thin film solar cells and how it is simulated.

## 1. Sun

The sun is a big sphere of gases that emits light and energy toward our planet. This energy received from the sun is a form of radiation also known as electromagnetic radiation. It is a distant star among many other stars, with a diameter of 1390000 km, it is composed of 80% hydrogen,19% helium, and 1% admixture of 100 other elements, and it is full of flammable gases, which represent more than 99.8% of the total mass of our solar system.[1, 2]

## 2. Solar energy

Solar energy is the term of the energy collected from solar irradiance, this energy can be converted into heat (thermal energy). Solar energy can be changed into chemical energy by plants ( photosynthesis ), or it can be used to generate electricity. The total solar energy that the world receives is far larger than all of its present and projected energy needs, if it used well, it would meet all of our energy demands. In contrast to typical energy sources, solar energy has recently emerged as one of the most popular and environmentally safe alternatives, indicating that it will last millions or perhaps billions of years.[2]

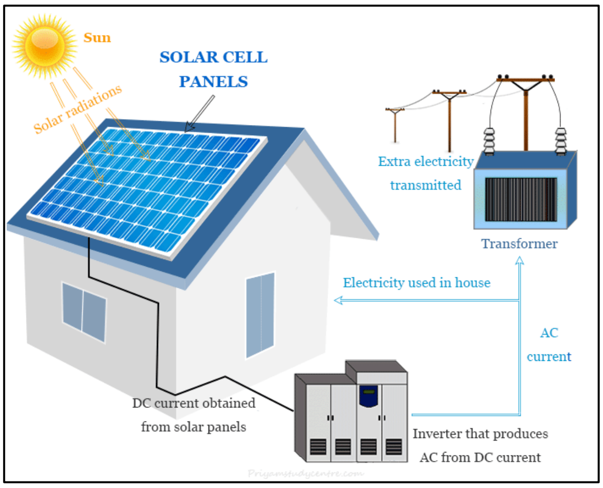


Figure 1 : Solar energy

# 3. Solar radiation

## 3.1. Types of solar radiation :

There are three types of solar radiation

### 3.1.1. Direct radiation (S):

It is the beam that crosses the atmosphere without reflection or scattering; it is a direct beam of light from the sun and remains unchanged without loss.

### 3.1.2. Diffuse radiation (D) :

It is the radiation subjected to scattering by the components of the atmosphere.

### 3.1.3. Total radiation (G):

It is the radiation reaching a point on the Earth's surface resulting from the sum of direct, diffuse, and reflected radiation.[3]

## 3.2. Spectrum of solar radiation :

The sun emits electromagnetic rays, and decomposing them into different wavelengths gives what is called: the electromagnetic spectrum, as it consists of all radiations of different colors, which are characterized by the wavelength range, and the frequency of light determines its color.

Photons, the grains of light that make up this radiation, are carriers of energy, which is related to frequency (wavelength) by the following relationship.[1]

$$E = h\upsilon = h\frac{c}{\lambda} \qquad (1)$$

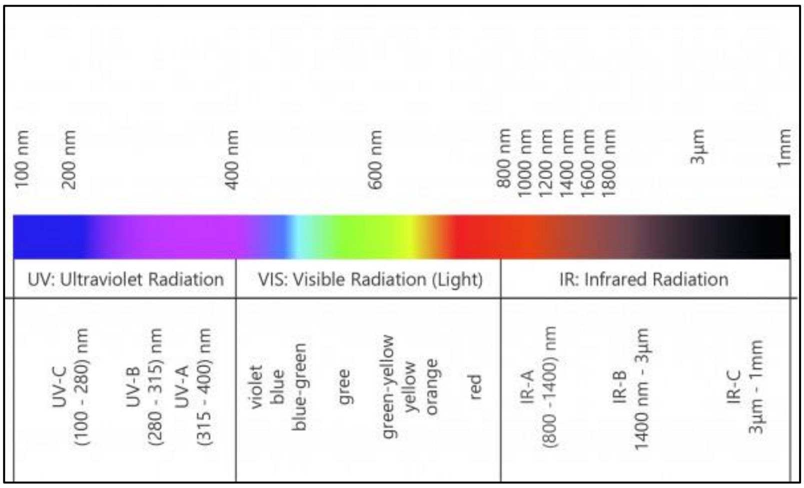


Figure 2 : Solar radiation spectrum

Table 1 : Approximate wavelengths of different colors in space

| visible light Spectrum | |
|---|---|
| Color | Wavelength (nm) |
| Red | 622-780 |
| Orange | 597-622 |
| Yellow | 577-597 |
| Green | 492-577 |
| Blue | 455-492 |
| Purple | 390-455 |

## 4. Conductors, insulators, and semiconductors :

### 4.1. Conductors :

In Electrical & Electronics engineering, a conductor is a type of material that allows the flow of charge otherwise known as electrical current. Most common electrical conductors are made from metals. Such materials allow the current flow due to the presence of free electron or ions which starts moving when voltage is applied.

The conductors have very low electrical resistance i.e. the opposition to the current flow & depend on the length & width of the conductor. It increases with increase in temperature.[4]

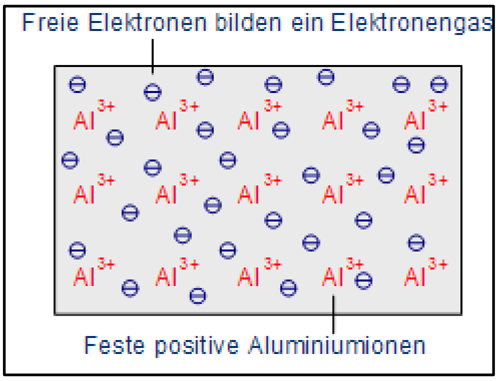


Figure 3 : Metallic bonding: fixed ions and free valence electrons (Fermi gas)[5]

### 4.2. Insulators :

An insulator is a material that has very high electrical resistance & it does not allow the flow of current. There are no free electrons in insulators thus they do not conduct electricity. Thus they are used for protection against shock.[4]

### 4.3. Semiconductors :

Semiconductors are materials that have conductivity in-between conductors and insulators. They can block or allow the current flow providing total control over it. They are mostly modified by adding impurities called doping. It modifies its properties like unidirectional current flow or amplification or energy conversion etc.[4]

The electrical conduction inside semiconductors is due to the movement of electrons & holes.

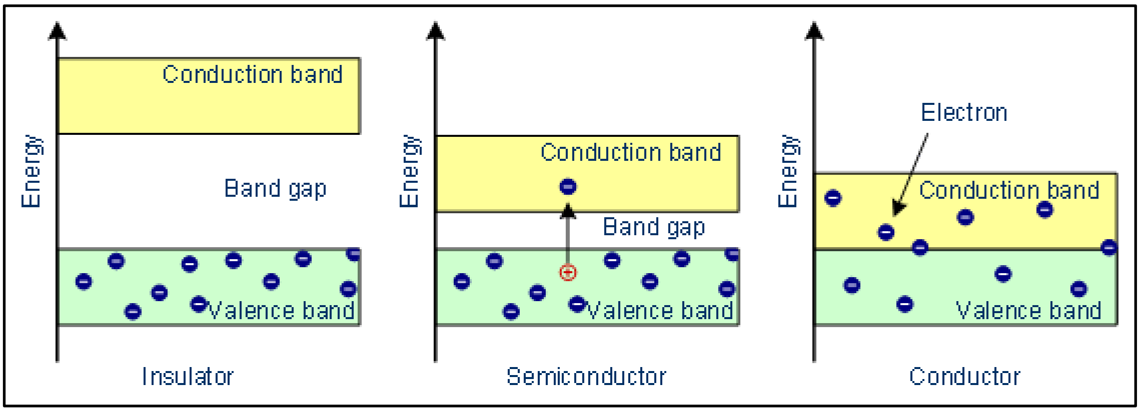


Figure 4 : The band model [5]

## 5. Elctrons and holes :

An electron hole is one of the two types of charge carriers that are responsible for creating electric current in semiconducting materials. A hole can be seen as the "opposite" of an electron. Unlike an electron which has a negative charge, holes have a positive charge that is equal in magnitude but opposite in polarity to the charge an electron has.

Holes are formed when electrons in atoms move out of the valence band (the outermost shell of the atom that is completely filled with electrons) into the conduction band (the area in an atom where electrons can escape easily), which happens everywhere in a semiconductor[6].

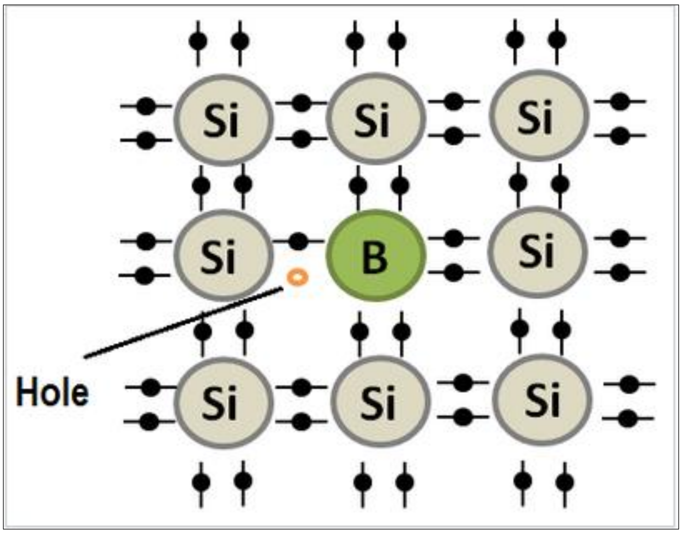


Figure 5 : A diagram showing a crystal lattice and how the movement of an electron from the valence band creates a hole

## 6. Doping :

Doping means the introduction of impurities into a semiconductor crystal to the defined modification of conductivity. Two of the most important materials silicon can be doped with, are boron (3 valence electrons = 3-valent) and phosphorus (5 valence electrons = 5-valent). Other materials are aluminum, indium (3-valent) and arsenic, antimony (5-valent).

The dopant is integrated into the lattice structure of the semiconductor crystal, the number of outer electrons define the type of doping. Elements with 3 valence electrons are used for p-type doping, 5-valued elements for n-doping. The conductivity of a deliberately contaminated silicon crystal can be increased by a factor of $10^6$.[7]

### 6.1. N-doping :

The dopants are positively charged by the loss of negative charge carriers and are built into the lattice, only the negative electrons can move. Doped semimetals whose conductivity is based on free (negative) electrons are n-type or n-doped. Due to the higher number of free electrons those are also named as majority charge carriers, while free mobile holes are named as the minority charge carriers [7].

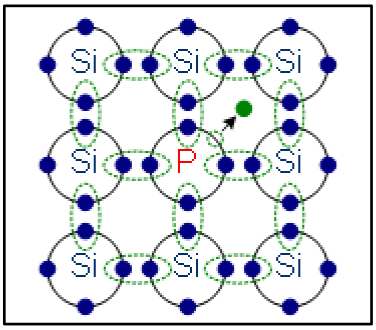


Figure 6 : N-doping with phosphorus

### 6.2. P-doping :

In contrast to the free electron due to doping with phosphorus, the 3-valent dopant effect is exactly the opposite. The 3-valent dopants can catch an additional outer electron, thus leaving a hole in the valence band of silicon atoms. Therefore the electrons in the valence band become mobile. The holes move in the opposite direction to the movement of the electrons. The necessary energy to lift an electron into the energy level of indium as a dopant, is only 1 % of the energy which is needed to raise a valence electron of silicon into the conduction band.[7]

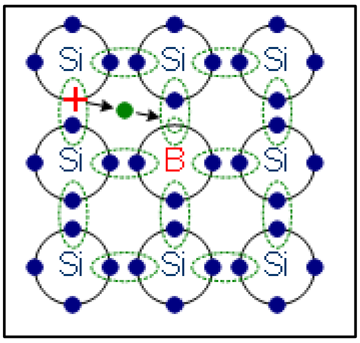


Figure 7 : P-doping with boron

## 7. P-N jonctuion :

The p-n junction is the transition area between two n- and p-doped semiconductor crystals. In this area there are no free charge carriers, since the free electrons of the n-conductor, and the holes of the p-doped crystal in the vicinity of the interface recombine with each other, which means that the electrons fill the holes. This charge movement (diffusion) is obtained in consequence of a concentration gradient: since there is only a few number of electrons in the p-area and only a few number of holes in the n-region, the majority charge carriers (electrons in the n-crystal, holes in the p-crystal ) move into the contrary doped semiconductor. The crystal lattice at the interface must not be interrupted, a simple "pressing together" of a p-type and a n-doped silicon crystal does not allow a functional p-n junction.[8]

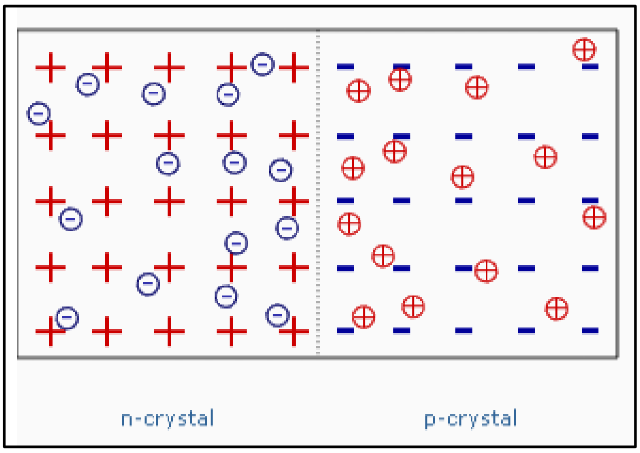


Figure 8 : P-N junction

## 8. Solar cells

### 8.1. Definition :

A solar cell in a basic term is a semiconductor diode that has been carefully designed to generate power from the sunlight. A diode is a single crystal semiconductor material such as silicon, having one side doped with pentavalent impurities forming n-type and anotherside doped with trivalent impurities as p-type.[9]

### 8.2. Working principles of solar cell :

The working principle of solar cells is based on the photovoltaic effect. The PV effect can be divided into three essential procedures

1. Absorption of photons in a p-n junction electronic semiconductor to generate the charge carriers (electron-hole pairs). The absorption of a photon with energy ($E = h\upsilon$) higher than the gap energy '$E_g$' of the doped semiconductor material means that its energy is used to excite an electron from the valence band '$E\upsilon$' to the conduction band '$E_c$' leaving a void (hole) at the valance level. Additional kinetic energy is given to the electron or hole by the excess photon energy ($h\upsilon – h\upsilon_0$). '$h\upsilon_0$′ is the minimum energy or work function of the semiconductor required to generate an electron-hole pair. The work function here represents the energy gap. The excess energy is dissipated as heat in the semiconductor.
2. Consequent separation of the light-generated charge carriers. In an external solar circuit, the holes can flow away from the junction through the p-region, and electrons

can flow out across the n-region and pass through the circuit before they recombine with the holes.

3. Finally, the separated electrons can be used to drive an electric circuit. After the electrons passed through the circuit, they will recombine with the holes.[9]

## 8.3. Different generations of solar cells :

### 8.3.1. First generation of solar cell :

Silicon-based PV cells were the first sector of photovoltaics to enter the market, using processing information and raw materials supplied by the industry of microelectronics. Solar cells based on silicon now comprise more than 80% of the world's installed capacity and have a 90% market share. Due to their relatively high efficiency, they are the most commonly used cells. The first generation of photovoltaic cells includes materials based on thick crystalline layers composed of Si silicon. This generation is based on mono-, poly-, and multicrystalline silicon, as well as single III-V junctions (GaAs).[10]

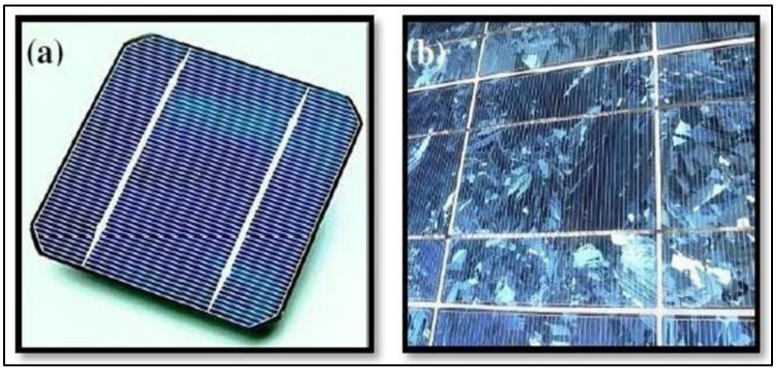


Figure 9 : (a) monocrystalline and (b) polycrystalline cells

### 8.3.2. Second generation of solar cell :

The thin film photovoltaic cells based on CdTe, gallium selenide, and copper (CIGS) or amorphous silicon have been designed to be a lower-cost replacement for crystalline silicon cells. They offer improved mechanical properties that are ideal for flexible applications, but this comes with the risk of reduced efficiency. Whereas the first generation of solar cells was an example of microelectronics, the evolution of thin films required new methods of growing and opened the sector up to other areas, including electrochemistry.[10]

Figure 10 : CIGS cells

### 8.3.3. Third generation of solar cell :

The third generation of solar cells (including tandem, perovskite, dye-sensitized, organic, and emerging concepts) represent a wide range of approaches, from inexpensive low-efficiency systems (dye-sensitized, organic solar cells) to expensive high-efficiency systems (III-V multi-junction cells) for applications that range from building integration to space applications. Third-generation photovoltaic cells are sometimes referred to as “emerging concepts” because of their poor market penetration, even though some of these have been studied for more than 25 years.[10]

Figure 11 : Organic solar cells

Table 2 : Types of solar cells[2]

| Generation | Type | Efficiency | Advanteges | Disadvantges |
|---|---|---|---|---|
| First Generation | Monocrystalline silicon | Up to 24% | * High efficiency<br>* Long lifetime | * High cost |
| | Polycrystalline silicon | 13–20% | * Lower cost | * Lower efficiency |
| Second Generation | Amorphous silicon | 5–10% | * Lower cost<br>* Flexible<br>* Ease of production | * Shorter lifetime<br>* Lower efficiency |
| | Cadmium telluride | 18–22% | * Lower cost<br>* High absorption | * Toxic |
| | Copper indium gallium diselenide | 15–22% | * Higher heat resistance | * Higher cost |
| Third Generation | Organic PV | Up to 17% | * Lightweight<br>* Eco-friendly | * Lower efficiency<br>* Shorter lifetime |
| | Concentrated PV | 40% | * Very high efficiency<br>* Can withstand high temperatures | * Very high cost<br>* Must be integrated with solar tracking systems and cooling devices to reach high efficiency |

### 8.4. Thin-film solar cells :

Thin film cells considered as 2nd generation cells. In general, this type of cell consists of two types which are based on a-Si silicon and also polycrystalline semiconductors like CIGS and CdTe. Today, the various deposition techniques (CVD) offer great flexibility for the manufacture of semiconductors.

The basic requirement is that the thickness of the thin film is greater than the absorption coefficient, so the greatest amount of light can be absorbed because the thin film solar cells made by semiconductor compositions with a direct gap and high absorption.[11]

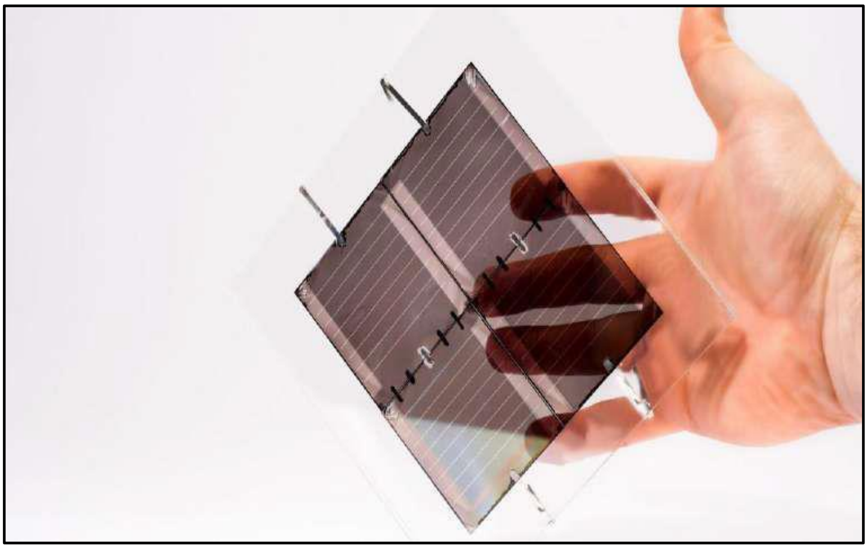

Figure 12 : Thin film solar cell

### 8.4.1. Types of thin film solar cells :

**Amorphous, micro/ nanocrystalline and polycrystalline silicon (a-Si) :**

Amorphous silicon is widely accepted as a thin-film solar cell material because: (a) it is abundant and non-toxic; (b) it requires low process temperature, enabling module production on flexible and low cost substrates; (c) the technological capability for large-area deposition exists; and (d) material requirements are low, 1–2 mm, due to the inherent high absorption coefficient compared with crystalline silicon.[12]

**Cadmium telluride (CdTe) :**

Owing to its optoelectronic and chemical properties, CdTe is an ideal absorber material for high efficiency, low cost thin film polycrystalline solar cells. CdTe is a direct band gap material with an energy gap of 1_5 eV, and an absorption coefficient _105/cm in the visible region, which means that a layer thickness of a few micrometers is sufficient to absorb _90% of the incident phtons. Owing to the high temperature of deposition in most cases, the films are deposited with Cd deficiency, giving rise to p-type conductivity. Because of the high ionicity (72%) of CdTe, the crystallite formed are well-passivated and strong chemical bonding (5_75 eV) results in high chemical and thermal stability.[12]

**Copper indium gallium diselenide (CIGS) :**

The I–III–VI chalcopyrite materials have some very desirable properties for photovoltaic application. CuInS2, having a band gap of 1.53 eV is considered an ideal material for photovoltaic application. The difficulties in controlling the sulfur during deposition and the relatively rapid diffusion of metals and impurity species, even at low temperatures, slow down the development of this material.61 However, devices with efficiency 11.4% have been reported.[12]

### 8.4.2. Components of thin films solar cells :

**Window layer :**

In thin film solar cells, the semiconducting material that form the window layer has the largest band gap of all the thin films making up the solar cell. The large band gap ensures that the window layer is transparent to most photons in the visible region of the solar spectrum. Most of the incident photons in this region will be transmitted by the window layer to the underlying layers of the solar cell, which ensures that the most photon absorption happens in the absorber layer.[13]

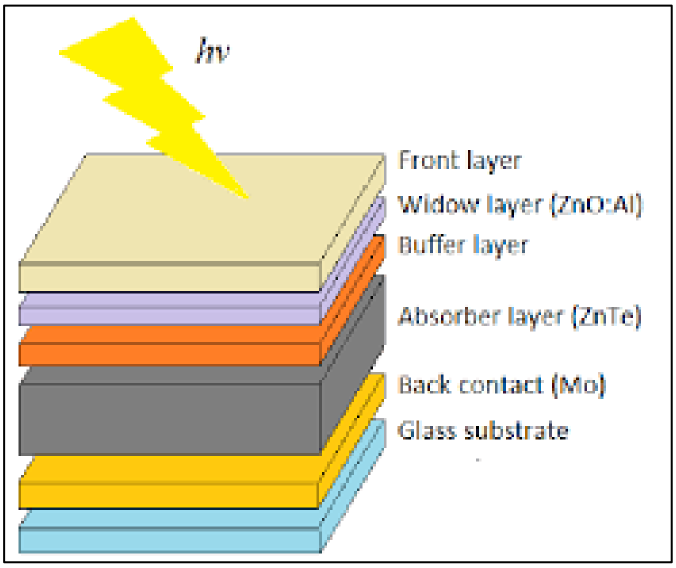


Figure 13 : Different layers of thin film solar cell

**ETL and HTL layers : (Electron Transport Layer and Hole Transport Layer)**

The ETL is the layer through which electrons move from mesoscopic perovskite and the conventional nanoparticles of mesoporous metal oxides like $TiO_2$ and ZnO, while holes are efficiently transported through a variety of HTLs. The perovskite absorber is supported by these layers significantly, but the thickness, carrier concentration, and associated bulk defects need to be adjusted to obtain the best cell performance with superior stability.[14]

**Absorber layer :**

The absorber layer is a semiconducting material often considered the heart of all thin film solar cells. It is aptly named because it is the layer that absorbs the highest number of photons and in response excites electrons into the conduction band to create photocurrent. Due to this, the absorber layers of all thin film solar cells are selected from semiconducting materials with band gap energies that coincide with the photon-rich region of the solar spectrum.[13]

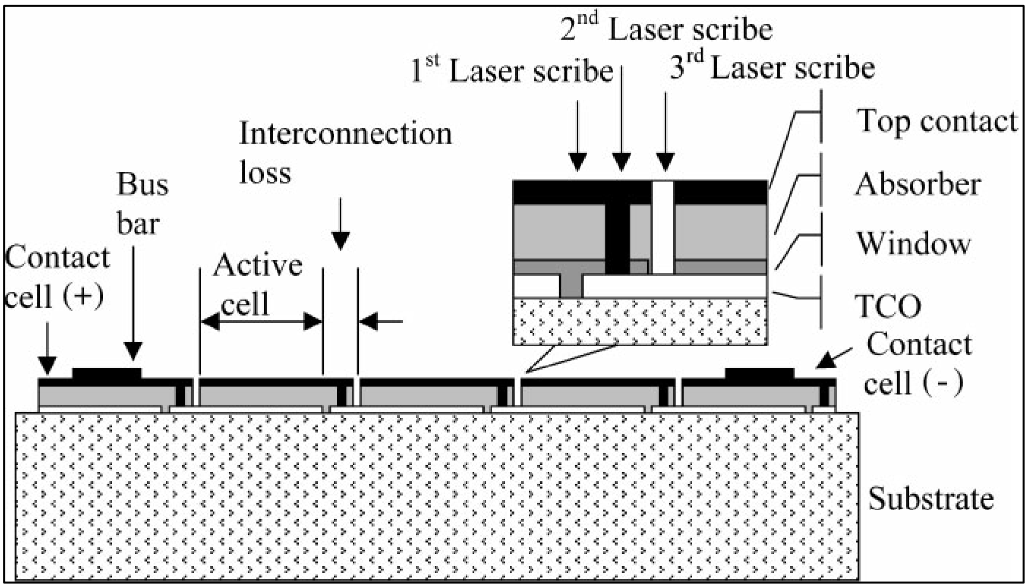


Figure 14 : Components of thin films solar cells :

### 8.5. Components of Solar Power System :

A PV system is composed of a solar panel, super capacitor, and inverter. The solar panel absorbs photon energy and transforms it into electricity through the PV mechanism. The super capacitor backup is used to deliver additional energy only on sunny days. The generated DC power is transformed into AC loads to be appropriate for domestic use[9]

### 8.6. Electrical characteristics of solar cells :

#### 8.6.1. Open-circuit voltage (Voc) :

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 for I=0 and VT=KT/q as the thermal potential, the expression for $V_{oc}$ is as follows.[15]

$$V_{oc} = V_{th}.\ln\left(\frac{I_{ph}}{Is}+1\right) \tag{2}$$

$$V_{th} = \frac{nkT}{q} \tag{3}$$

$V_{th}$ : thermodynamics voltage.

#### 8.6.2. Short circuit current $I_{sc}$ :

It is the maximum current produced by the cell that is measured when there is no resistance in the circuit, it is obtained when the circuit is short and the produced capacity is non-existent because the value of the voltage in this case is zero.[16]

$$I_{sc} = \frac{I_{ph}}{1+\frac{R_s}{R_{sh}}} \tag{4}$$

#### 8.6.3. 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.[15]

The maximum power delivered to the charge is given by the expression :

$$P_{max} = V_{max}.I_{max} \tag{5}$$

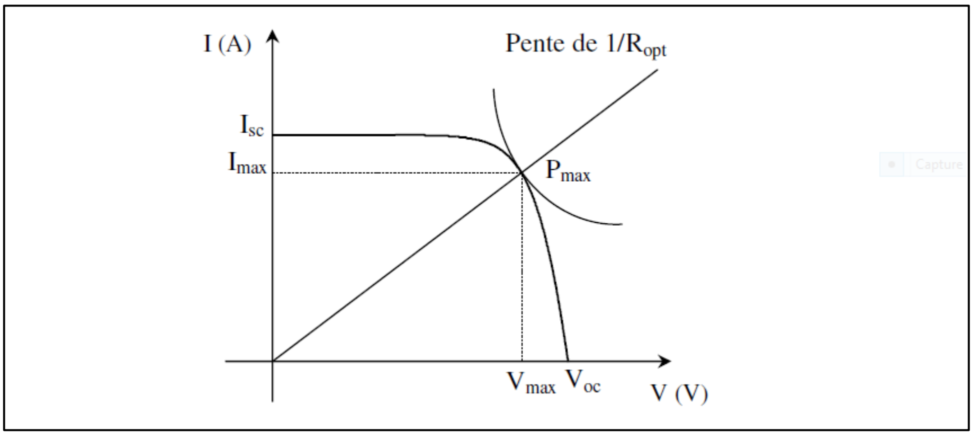


Figure 15 : Maximum power point of a single atomic cell

### 8.6.4. Fill factor FF :

The FF form, also known as fill factor it is defined by:

$$FF = \frac{P_{\max}}{P_{\max ideale}} = \frac{V_{\max}.I_{\max}}{V_{oc}.I_{sc}} \quad (6)$$

This factor shows the deviation of the curve I = f (V) from a rectangle (of length Vco and width Isc) which corresponds to the ideal solar cell.[17]

### 8.6.5. 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:

$$\eta = \frac{P_{\max}}{P_{in}} = \frac{V_{\max}.I_{\max}}{P_{in}} = \frac{V_{oc}.I_{sc}.FF}{ES} \quad (7)$$

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]

### 8.7. Curves of solar cell :

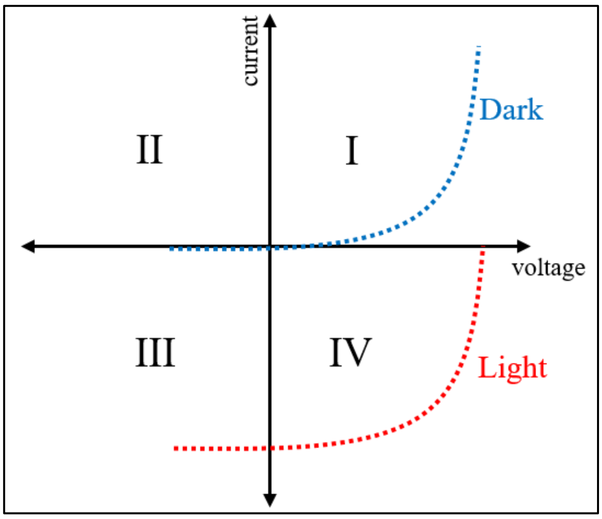


Figure 16 : Dark and light IV curves for an OPV

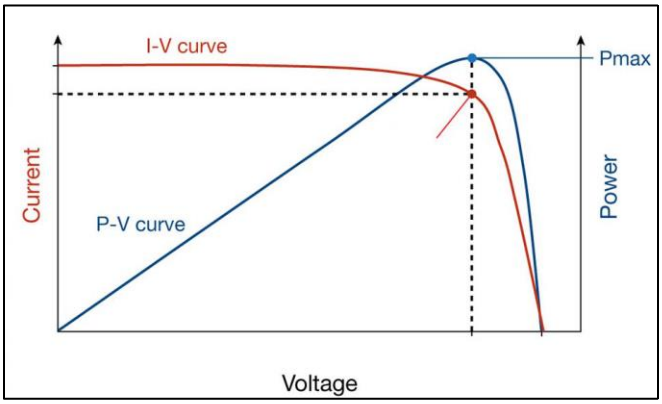


Figure 17 : I-V curve and maximum power point

## 9. Simulation of solar cell

### 9.1. Solar Cell Characterizations :

The solar cell in the dark acts as a simple diode, and the equivalent electric circuit that approximates it is shown in figure which comprises:

1. A diode with $I_D$ current (current in the dark reverse bias).

2. A current source that corresponds to photocurrent $I_L$ generated during illumination.

3. $R_s$ series resistance.

4. $R_{sh}$ shunt resistance with $I_{sh}$ leakage current through resistance as a result of defects in the films.[18]

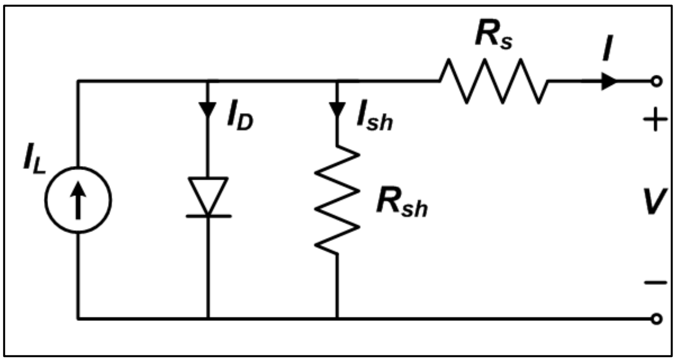


Figure 18 : Equivalent circuit for OPV

### 9.2. Single diode and double diode PV cell :

#### 9.2.1. Ideal solar cell :

If the characteristic of the junction is of the form:

$$I_D = I_s\left(e^{\frac{qV}{nkT}} - 1\right) \tag{8}$$

We can admit that in the presence of light, there is appearance of an additional photocurrent, $I_{ph}$ whose direction is opposite to the direct current. By connecting an external circuit to the solar cell, this current is collected. The current under light is :

$$I = I_{ph} - I\left(e^{\frac{V}{nkT}} - 1\right) \tag{9}$$

#### 9.2.2. Single-diode PV cell model:

A solid, single-junction PV cell that is not illuminated behaves very similarly to a semiconductor diode. The conventional equation below describes a simple diode with a distinctive I–V curve:

$$I_D = I_0\left[\exp\left(\frac{qV_D}{nkT} - 1\right)\right] \tag{10}$$

The ideality factor (quality factor or emission coefficient), which usually ranges from 1to 2 but might be higher in certain cases, is determined according to the fabrication process and the semiconductor material. Given that n is generally assumed to be roughly equal to1,it is often left out. When the semiconductor diode is illuminated, it will produce a photo-generated current, $I_{ph}$, which will result in a vertical translation of the I–V curve of a quantity that is almost entirely related to the surface density of the incident energy. Thus, an ideal cell is depicted as a current generator that is linked to a parallel diode with an I–V characteristic, which is mathematically defined by Shockley in the following equation as [19] :

$$I = I_{ph} - I_0\left[\exp\left(\frac{qV_D}{nkT}\right) - 1\right] - \frac{V_D}{R_{sh}} \qquad (11)$$

Where : $V_D = V_{pv} + R_s I$

A simple theoretical definition is presented by Eq because it does not consider the impact caused by the presence of the electrodes, one above and another below the semiconductor layer, which are required to accumulate the charges that cover the intercepting surface to some extent.

### 9.2.3. Double-diode PV cell model :

the photocurrent in a PV cell is generated not only by a single diode but also by the overall effect of multiple elementary diodes that are adjacent to one another and consistently distributed along the surface between the two layers of the semiconductor. A current passes through each basic diode while flowing across the semiconductor layers a long a different path, marked by different electric resistance and reduction in voltage.

Wolf developed a simplified equivalent circuit, as shown in Fig19. This model consists only of double diodes, a current generator, and two resistors, taking into consideration the dissipative effects and the existence of any construction flaws. Their solution of the equivalent circuit resulted in the following implied expression of the circuit I [19]:

$$I = I_{ph} - I_{01}\left[\exp\left(\frac{qV_D}{n_1kT}\right) - 1\right] - I_{02}\left[\exp\left(\frac{qV_D}{n_2kT}\right) - 1\right] - \frac{V_D}{R_{sh}} \qquad (12)$$

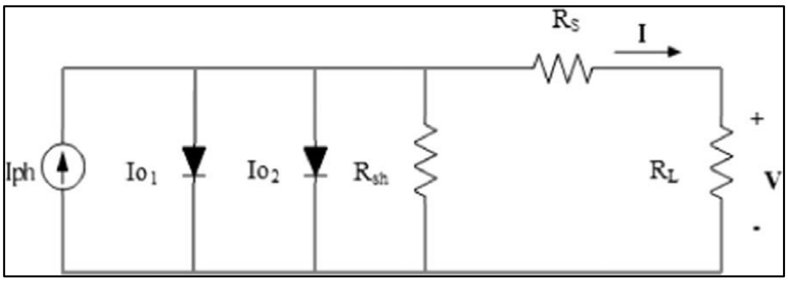


Figure 19 : Double-diode model equivalent circuit.

### 9.3. Concepts in solar cell simulation :

#### 9.3.1. Valence Band:

The valence band is the band of electron orbitals that electrons can jump out of, moving into the conduction band when excited.

#### 9.3.2. Conduction Band :

The conduction band is the band of electron orbitals that electrons can jump up into from the valence band when excited.

#### 9.3.3. Fermi Level :

The highest energy level that an electron can occupy at the absolute zero temperature is known as the Fermi Level. The Fermi level lies between the valence band and conduction band because at absolute zero temperature, the electrons are all in the lowest energy state.

#### 9.3.4. Fermi energy :

The Fermi energy is a concept in quantum mechanics usually referring to the energy difference between the highest and lowest occupied single- particle states in a quantum system of non-interacting fermions at absolute zero temperature.

#### 9.3.5. The electron affinity :

The electron affinity (E ea ) of an atom or molecule is defined as the amount of energy released when an electron attaches to a neutral atom or molecule in the gaseous state to form an anion. $X(g) + e^- \rightarrow X^-(g) + \text{energy}$. This differs by sign from the energy change of electron capture ionization. The electron affinity is positive when energy is released on electron capture.

#### 9.3.6. The work function :

The minimum amount of energy required to be provided to an electron to pull it out of the metal from the surface is called the work function of the metal.

#### 9.3.7. Band gap :

A band gap is the distance between the valence band of electrons and the conduction band.

#### 9.3.8. Band diagram :

A band diagram helps to explain the operation of semiconductor devices. It is a diagram where various key electron energy levels are plotted as a function of some spatial dimension.

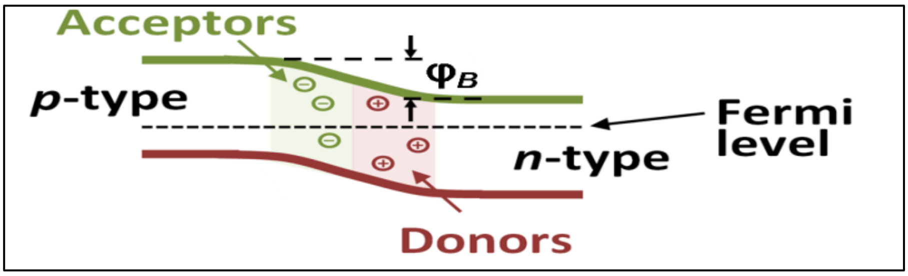


Figure 20 : Band diagram

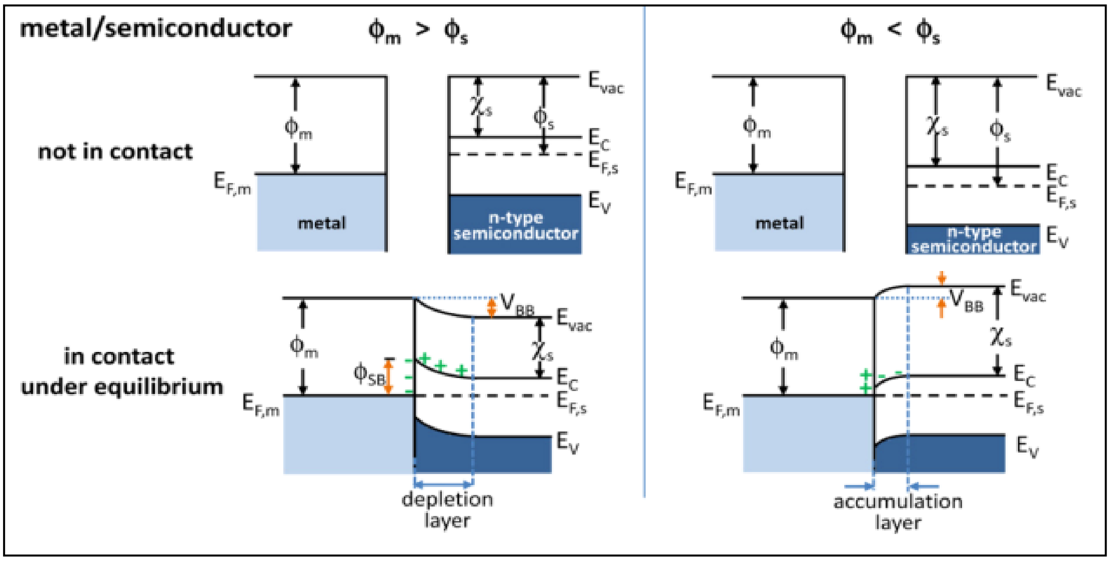


Figure 91 : Energy band diagrams of the surface contact between metals and n-type semiconductors. The vacuum energy, the maximum energy of the valence band , minimum energy of the conduction band, the metal work function , the semiconductor work function

## Conclusion

Solar radiation and the majority of the ideas pertaining to solar cells were covered in this chapter. We clarified the properties of the solar cell by talking about the different varieties, the mechanism of action, and the components. We also concentrated on a particular kind of solar cell in our work, known as thin film solar cells.

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# Chapter 02 :

# SCAPS-1D program

## Introduction

Nanotechnology has become the world attention in various applications including the solar cells devices due to the uniqueness and benefits of achieving low cost and better performances of devices. Recently, thin film solar cells such as Cadmium Telluride (CdTe), Copper-Indium-Gallium-diSelenide(CIGS), Copper-Zinc-Tin-Sulphide (CZTS), and Dye-Sensitized Solar Cells (DSSC) enhanced by nanotechnology have attracted much attention [1].In this chapter, we will learn about the simulation program SCAPS 1D and how to use this program. Multiple comprehensive studies on the structure design and characterization of solar cells are included in SCAPS. In this work we will simulate CdTe, CIGS and CZTS thin film solar cell using solar cell capacitance simulator (SCAPS).

## 1. Fundemental equations in semiconductors :

Semiconductors physics is an area very rich in modeling and mathematics problems. It consists of a fundamental set of equations that bring together electrostatic potential and load carriers in a very specific field of simulation. These equations, which are resolved via specific software for simulating semiconductor-based devices, are derived from Maxwell equations.[2]

They are mainly: Poisson's equation and continuity equations for both electrons and holes given by the following equations, which are used by SCAPS [2]:

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{q}{\varepsilon}\left[p(x) - n(x) + N_D - N_A + \rho_p - \rho_n\right] = 0 \quad (1)$$

$$\frac{1}{q}\frac{dJ_p}{dx} = G_{op}(x) - R(x) \quad (2)$$

$$\frac{1}{q}\frac{dJ_n}{dx} = -G_{op}(x) + R(x) \quad (3)$$

$\varepsilon$ : the dielectric constant

$q$ : the electron charge

$N_A$ : acceptor density

$N_D$ : donor density

$\psi$ : the electrostatic potential

$p$ : hole concentration

$n$ : electron concentration

$\rho_p$ : hole distribution

$\rho_n$ : electron distribution

$J_p$ : current densities of hole

$J_n$ : current densities of electron

$G_{op}$ : the optical generation rate

R : the net recombination from direct and indirect recombination.

## 2. About the program :

SCAPS-1D is a powerful one-dimensional solar cell simulation software developed by M. Burgelman at the Department of Electronics and Information Systems, University of Gents, Belgium. SCAPS-1D allows us to design solar cell structures and analyse their electrical properties and spectral response. Moreover, it is capable of modelling multivalent defects and tunnelling effects, which are commonly observed in thin-film heterojunction solar cells. SCAPS-1D is based on solving the basic carrier semiconductor equations using finite differential methods.[3]

### 2.1. Definitions :

#### 2.1.1. Working point :

- The temperature T: relevant for all measurements. Note: in SCAPS, only $N_C(T)$ the effective conduction band density, $N_V(T)$ the effective valence band density, the electron and hole thermal velocities and all their derivatives are the only variables which have an explicit temperature dependence; you must input for each $T$ the corresponding materials parameters yourself.
- The voltage V: is discarded in I-V and C-V simulation. It is the dc-bias voltage in C-f simulation and in QE(λ) simulation. SCAPS always starts at 0 V, and proceeds at the working point voltage in a number of steps that you also should specify.
- The frequency f: is discarded in I-V, QE(λ) and C-f simulation. It is the frequency at which the C-V measurement is simulated.

- The illumination: is used for all measurements. For the QE(λ) measurement, it determines the bias light conditions. The basis settings are: dark or light, choice of the illuminated side, choice of the spectrum. A one sun ( = 1000 $W/m^2$) illumination with the ‘air mass 1.5, global’ spectrum is the default, but you have a large choice of monochromatic light and spectra for your specialized simulations. If you have an optical simulator at your disposal you can immediately load a generation profile as well in stead of using a spectrum. [4]

### 2.1.2. Series resistance/ shunt resistance :

It is possible to introduce an external shunt conductance and series resistance to the structure on the action panel, Both resistances can be switched on/off and for a shunt conductance you can either define its resistance or conductance.[4]

### 2.1.3. Illumination :

When performing simulations under illumination, you can further specify the illumination conditions. The basis settings are: dark or light, choice of the illuminated side, choice of the spectrum. If you have an optical simulator at your disposal you can immediately load a generation profile as well in stead of using a spectrum.[4]

### 2.1.4. Batch calculations :

When you want to explore the influence of one or a few parameters to the solar cell characteristics, you can take profit of the batch option. When you click ‘Batch set-up’, a panel opens where you can choose which parameter to vary, over which range, and in which mode (Lin, Log or custom). You can also define more than one parameter, and vary all of them (in a nested way or ‘simultaneous’). Now, up to nine batch parameters can be defined, but be modest to start. A batch calculation is launched when ‘calculate: batch’ is clicked. After a batch simulation all parameters on the panels are reset as they were before the calculation.[4]

### 2.1.5. Recorder calculations :

In a regular single shot or batch calculation, the detailed panels are only available for the last measurement point. To be able to see them as a function of the batch parameters you can launch a record calculation. You should first select the properties which you want to keep track of by clicking ‘Record set-up’. By clicking ‘calculate: recorder’, a recorder calculation is launched. Cell parameters are varied according to the Batch set-up, and all simulations (and only those) are performed which are needed to determine the asked properties. This means the selected measurements on the action panel are ignored! [4]

### 2.1.6. Curve fitting :

The purpose of curve fitting is to vary one or more parameters in the cell definition to obtain a fit between one or more measured curves and the simulation.[4]

### 2.1.7. Scripting :

SCAPS is and has been designed to be a user-interactive program. The most important computer should be based on neurons instead of on transistors. It is important that the user understands what is physically happening rather than performing more simulations than (s)he ever could analyze. Nevertheless, SCAPS also provides the possibility to write a script and run it.

There are several levels of sophistication for the SCAPS script. One can use it to create a personalized version of SCAPS, to automate actions within the user interface, to use SCAPS in symbiosis with another program, to run SCAPS without mouse-clicks.[4]

## 2.2.SCAPS action panel :

1-Run SCAPS.

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

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

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

5-Start the calculation(s) .

6-Display the simulated curves [5]

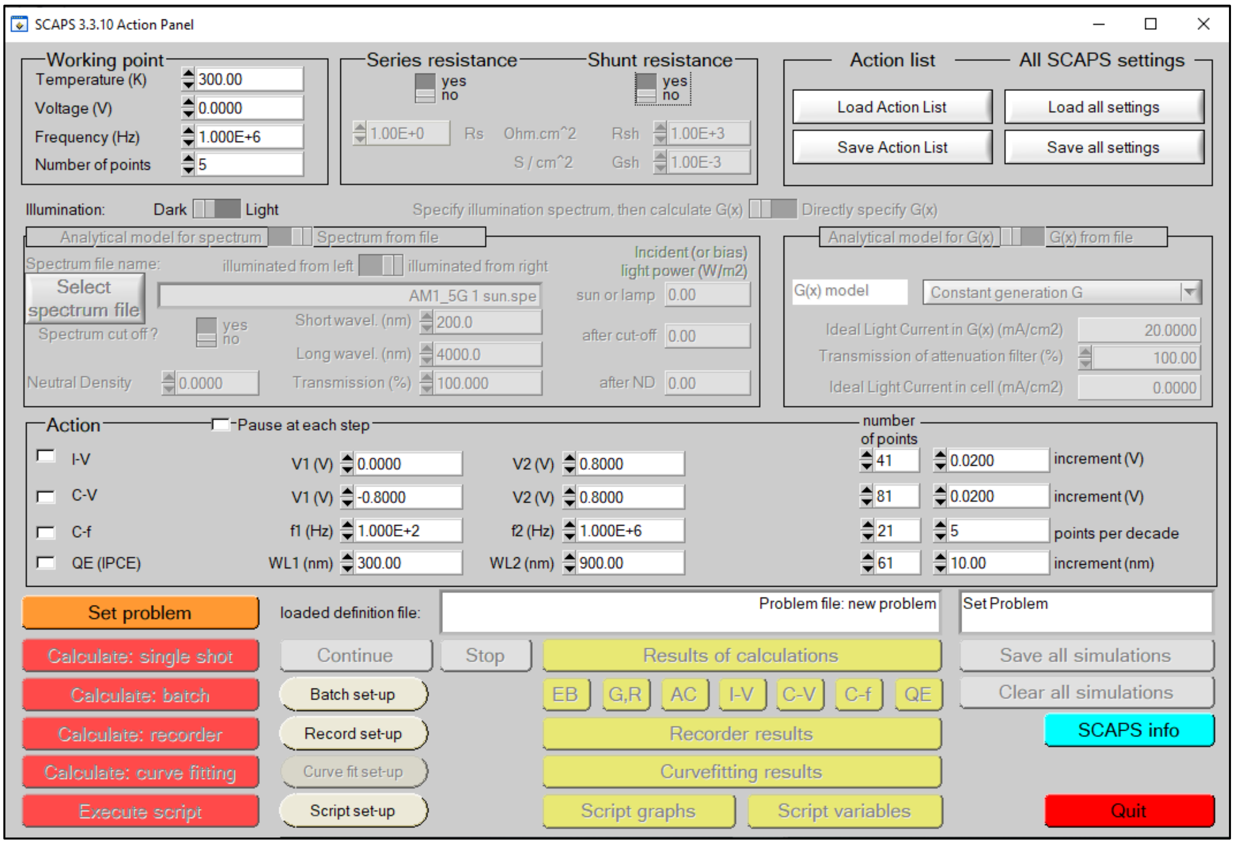
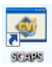
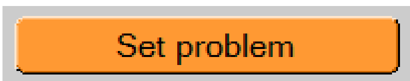



Figure 1 : SCAPS action panel

### 2.3.How to use SCAPS :

#### 2.3.1. Run SCAPS: 

Click the above pictogram on the Desktop. SCAPS opens with the Action Panel.

#### 2.3.2. Define problem : 


Click the button set problem in the action panel, and chose load in the lower right corner of the panel that opens. Select and open e.g. the file NUMOS CIGS baseline.def: that is the example problem file of the practicum session at the NUMOS workshop, Gent, 30 march 2007. This file is supposed to be in the folder / SCAPS /def, where / SCAPS / stands for the directory where you installed SCAPS, and where the SCAPS .exe file resides. If necessary, browse to find this file. In a later stage, you can alter all properties of the cell by clicking set problem in the action panel [4]. You can design your solar cell and change different layers by clicking on add layer and modify properties such us thickness, band gap.[4]

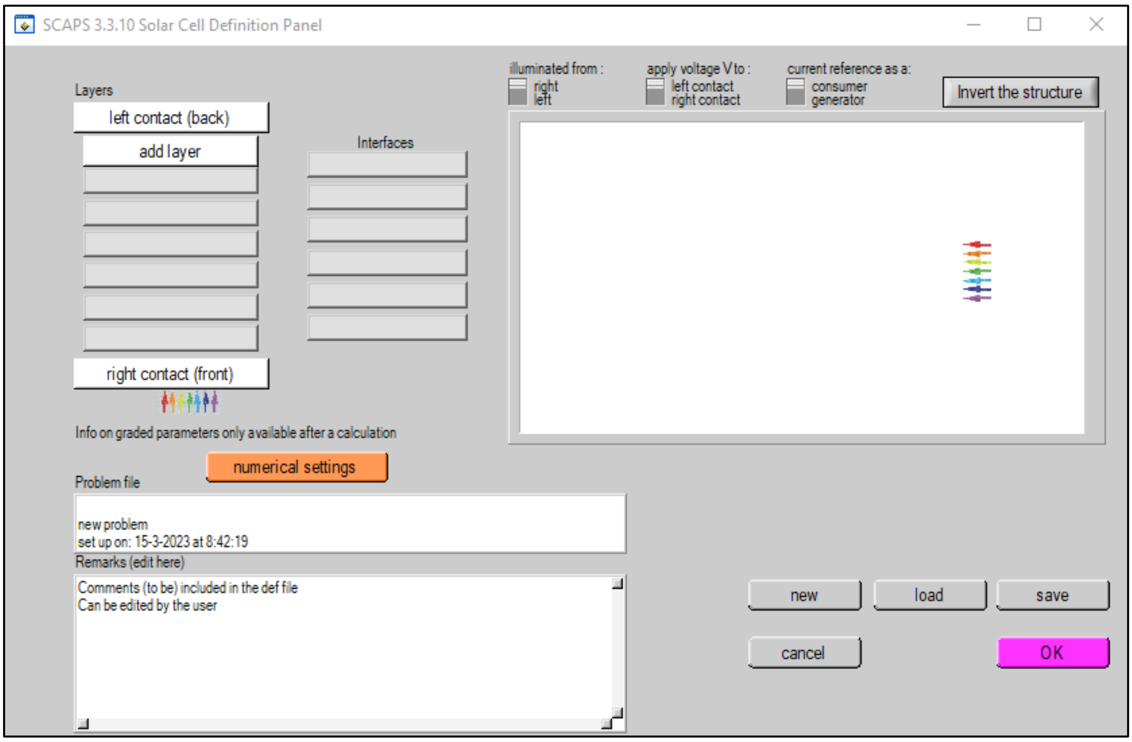



Figure 2 : SCAPS solar cell definition panel

### 2.3.3. Change parameters :

You can change parameters of different layers such as thickness, band gap, electron affinity… by clicking on the layer.

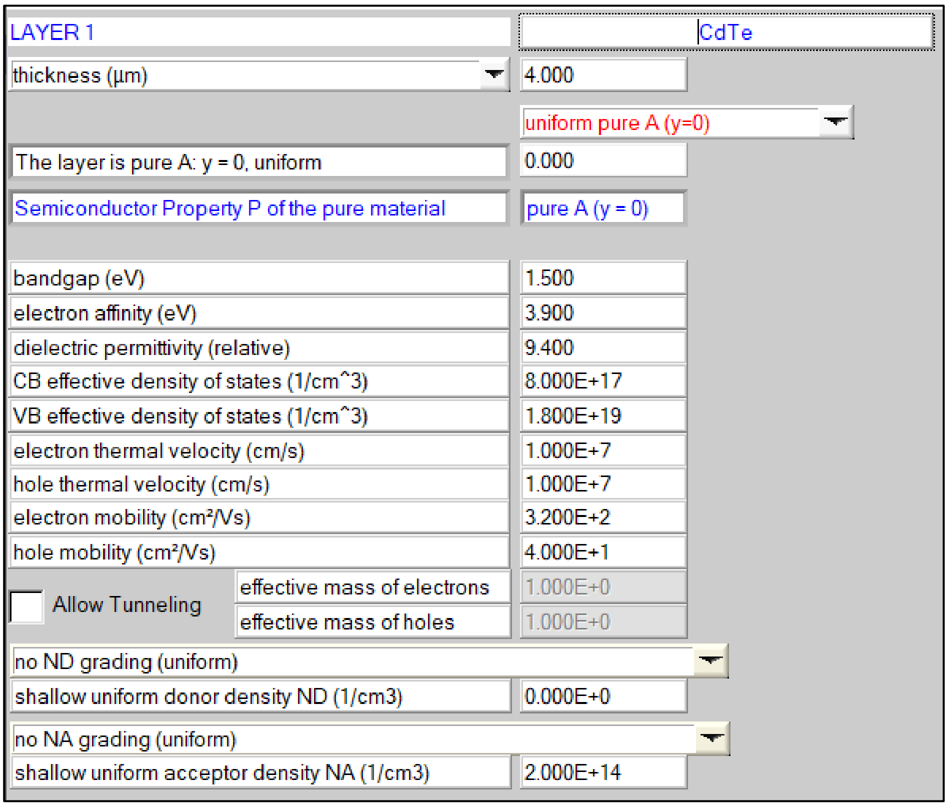



Figure 3 : Parameters of the layer

### 2.3.4. Define the working point :

The working point specifies the parameters which are not varied in a measurement simulation, and which are relevant to that measurement.

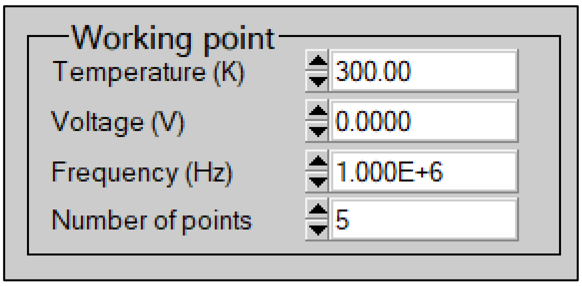



Figure 4 : SCAPS Working point

### 2.3.5. Spectrum and illumination :

Choose if you are simulating in dark or light, and select spectrum file you can find many files in SCAPS data base.

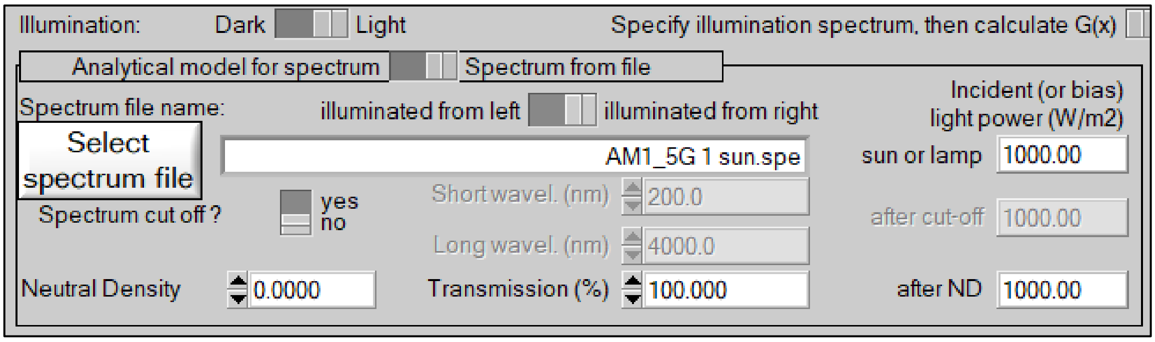


Figure 5 : SCAPS spectrum and illumination

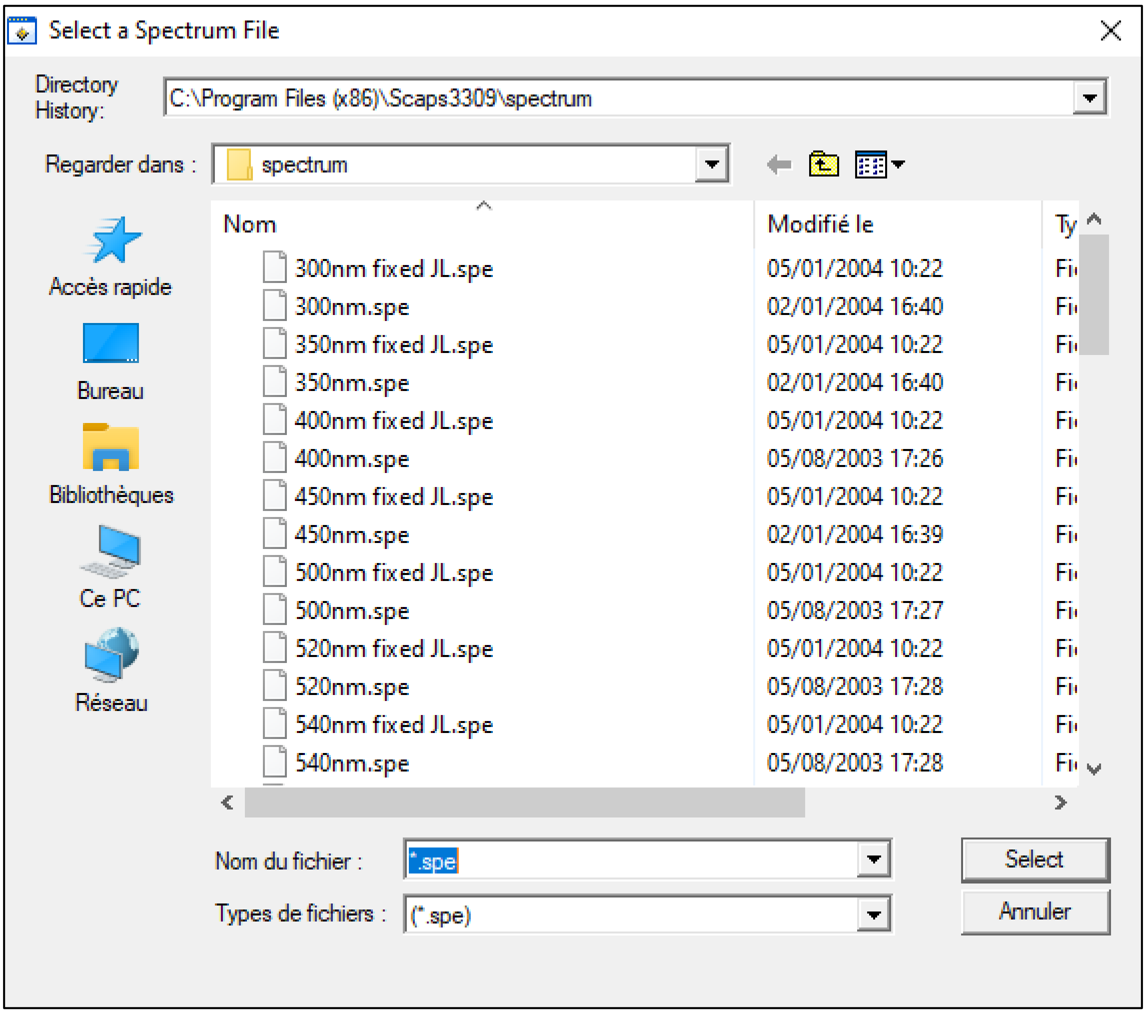


Figure 6 : Selecting Spectrum file

### 2.3.6. Select the measurements to simulate :

In the action-part of the Action Panel, you can select one or more of the following measurements to simulate: I-V, C-V, C-f and QE((λ). Adjust if necessary the start and end values of the argument, and the number of steps.[4]

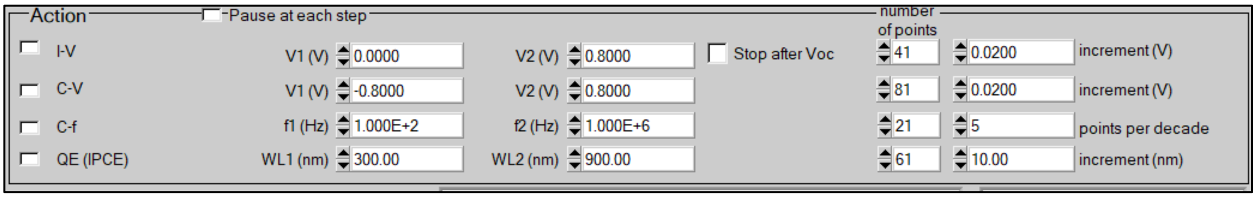



Figure 7 : Measurements panel

### 2.3.7. Start the calculation :


Click the button calculate: single shot in the action panel. The Energy Bands Panel opens, and the calculations start.

### 2.3.8. Display the simulated curves :

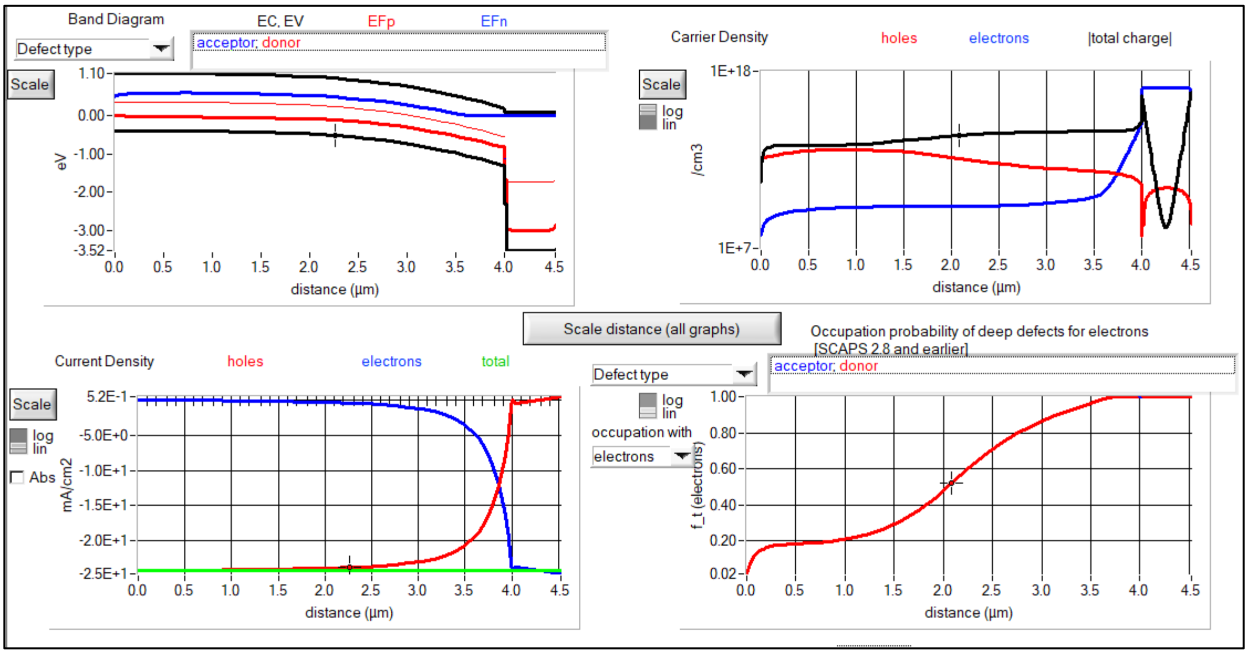



Figure 8 : SCAPS energy band panel

### 2.3.9. Batch recording panel :

After choosing batch and record set-up from action panel you can find results in calculate : recorder exactly in recorder.

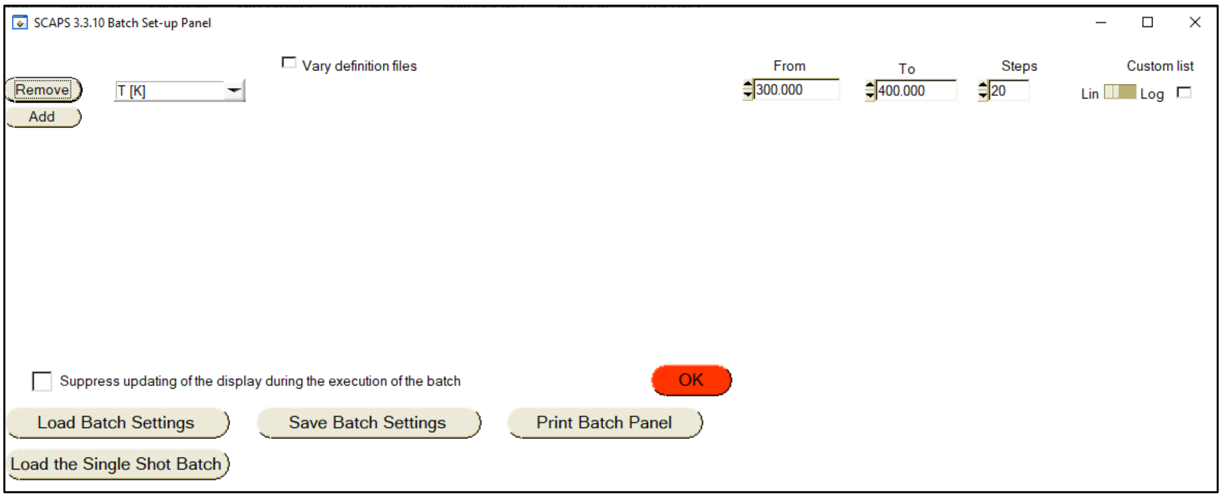



Figure 9 : Batch set-up panel

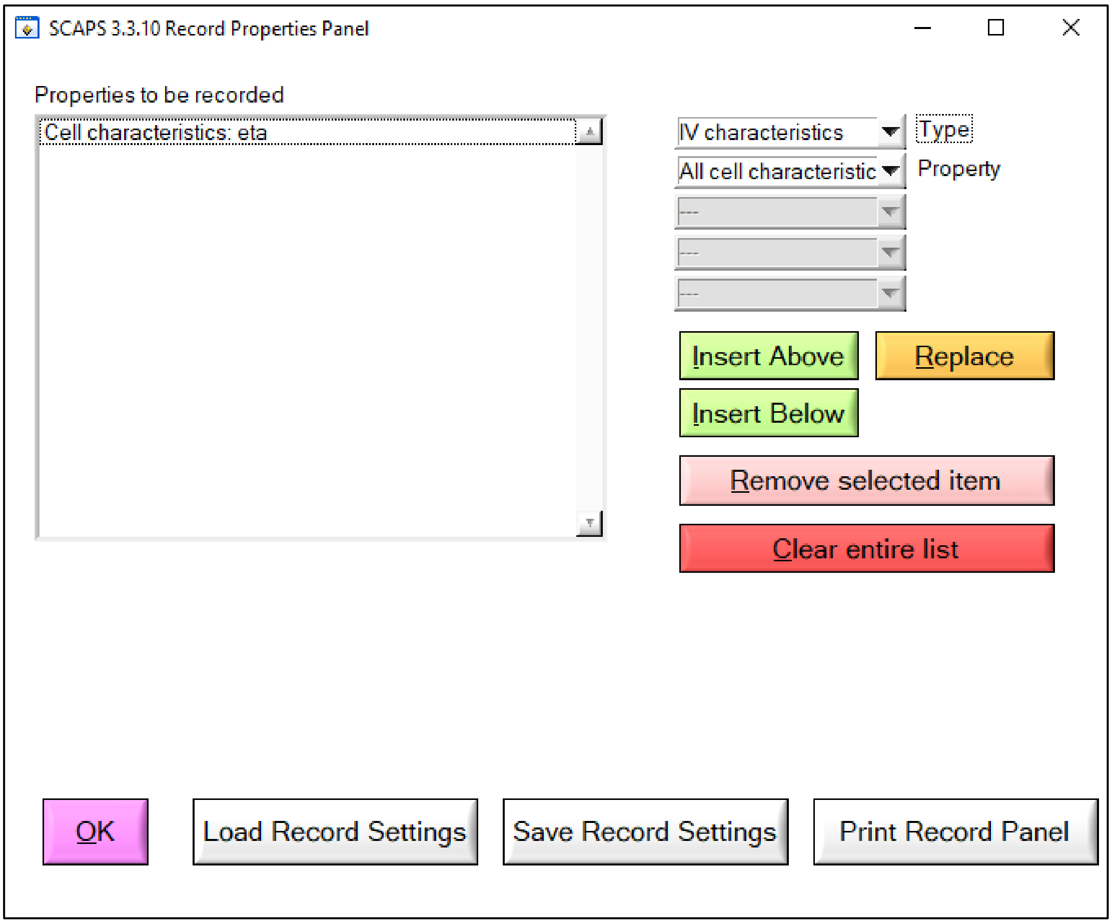



Figure 10 : Recorder properties panel

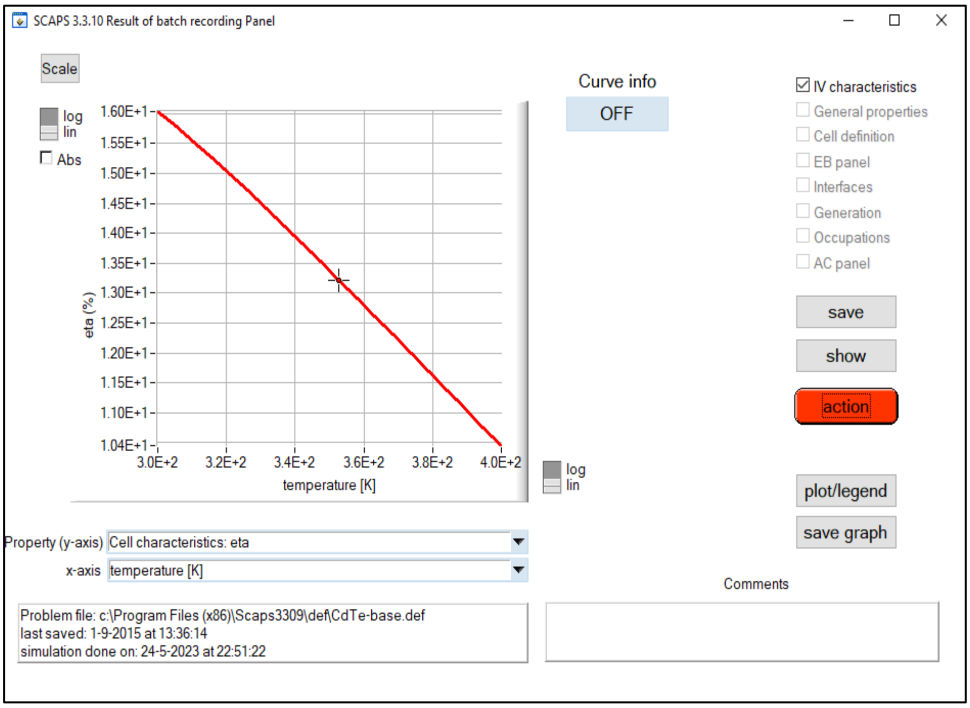



Figure 11 : Results of batch recording panel

Warning:

• Don't ask too many parameters at a time: the calculation could be much more time consuming than expected. When you have e.g. 3 nested parameters with each 6 values, you ask for 216 simulations…

• When it goes wrong, or goes too slow to your taste, or you are realizing too late that you were too ambitious, keep the SHIFT-key pressed, until the simulation stops. Your calculations done so far are not lost.

• Make smart use of the line /log key at the right hand end of each parameter line. Some parameters really ask for a variation on a log-scale (e.g. doping densities), others for a linear variation (e.g. a thickness).

Operating SCAPS in batch mode will save you much time, when it comes to explore the influence of a few parameters on a simulated measurement, e.g. the I-V curves. [6]

## Conclusion

In this chapter, we described SCAPS-1D simulation program. We started with introducing the fundamental equations in semiconductors which are used by SCAPS. We explained how to use necessary functions in this program and how to start simulating and finding results. Finally, we ended by warnings that should take into consideration while using SCAPS program.

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# Chapter 03 :

# Simulation results

## Introduction

This chapter is divided into three main parts, the first part is a simulation of a thin film solar cell from SCAPS database. The second part is a comparison between two simulated thin film solar cells using SCAPS-1D.The third part is a comparison between SCAPS-1D and AFORS-HET results.

## 1. Solar cell structure from SCAPS-1D database :

Figure.1 shows the CdTe/CdS/$SnO_2$ structure of the solar cell studied in this part. Table.1 shows some parameters of the selected solar cell simulated in this part, namely is CdTe-base.def with series resistance.

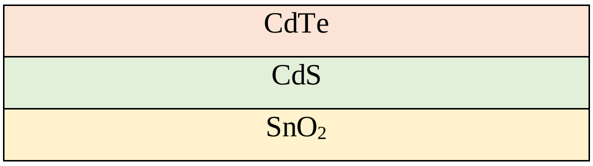
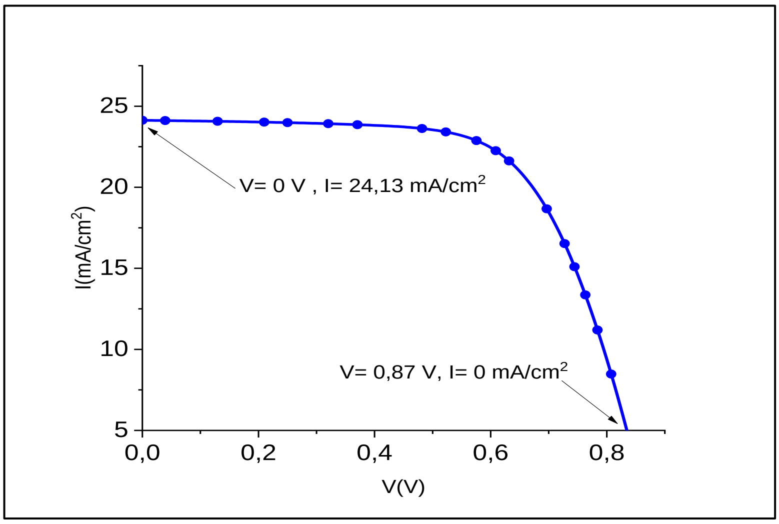



Figure 1 : The CdTe/CdS/$SnO_2$ structure of the studied solar cell in part1

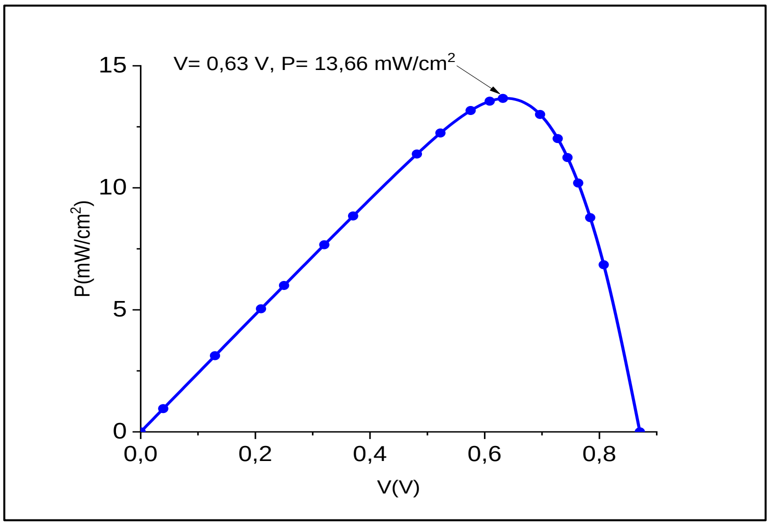
Table 1 : CdTe-base solar cell properties

| parameters | CdTe | CdS | $SnO_2$ |
|---|---|---|---|
| **Thickness (µm)** | 4.000 | 0.025 | 0.500 |
| **Band gap (eV)** | 1.500 | 2.4 | 3.600 |
| **Electron affinity (eV)** | 3.900 | 4.000 | 4.000 |
| **Dielectric permittivity (relative)** | 9.400 | 10.000 | 9.000 |
| **CB (cm$^{-3}$)** | 8.000E+17 | 2.2000E+18 | 2.200E+18 |
| **VB (cm$^{-3}$)** | 1.800E+19 | 1.800E+19 | 1.800E+19 |
| **Electron thermal velocity (cm/s)** | 1.000E+7 | 1.000E+7 | 1.000E+7 |
| **Hole thermal velocity (cm/s)** | 1.000E+7 | 1.000E+7 | 1.000E+7 |
| **Electron mobility (cm²/Vs)** | 3.200E+2 | 1.000E+2 | 1.000E+2 |
| **Hole mobility (cm²/Vs)** | 4.000E+1 | 2.500E+1 | 2.500E+1 |
| **Shallow uniform donor density ND (cm$^{-3}$)** | 0.000E+0 | 1.100E+18 | 1.000E+17 |
| **Shallow uniform acceptor density NA (cm$^{-3}$)** | 2.000E+14 | 0.000E+0 | 0.000E+0 |

## 1.1.I-V and P-V curves :




(a)




(b)

Figure 2 : a) I-V Current curve of the solar cell, (b) Power versus voltage of the $CdTe/CdS/SnO_2$ solar cell

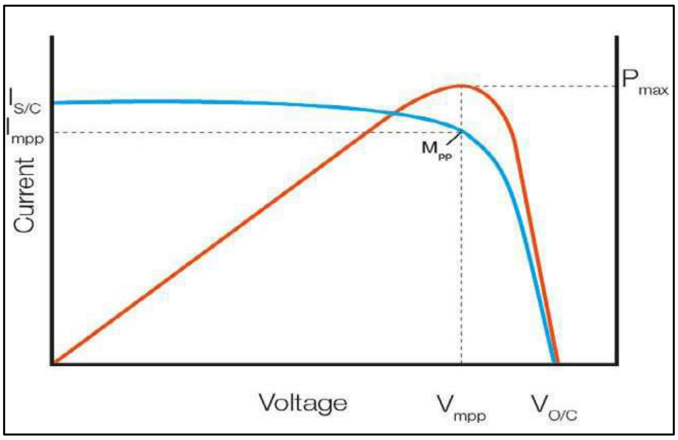



Figure 3 : Current and power curves of solar cell [1]

Simulation results shows that the current produced by the $CdTe/CdS/SnO_2$ solar cell when exposed to radiation is maximum in the case of short circuit with a value of $I_{sc}$ = 24.13 mA/cm$^2$. The cell current decreases slowly with the increasing of the voltage between its terminals up to 0.63V, then the decrease is significant until the absence of current at the open circuit voltage $V_{oc}$=0.87 V.

From the power curve, we notice an almost linear increase in the power values with the increase of the voltage until a maximum value $P_{max}$= 13.66 mW/cm$^2$, then the power decreases until zero at the open circuit voltage.

By analyzing the simulation results, we obtain the following solar cell characteristics:

Table 2 : Characteristics of the $CdTe/CdS/SnO_2$ solar cell

| | |
|---|---|
| Open circuit voltage $V_{oc}$ | 0.87 V |
| Short circuit current $I_{sc}$ | 24.13 mA/cm$^2$ |
| Maximum power point $P_{max}$ | 13.66 mW/cm$^2$ |
| Maximum voltage $V_m$ | 0.63 V |
| Maximum current $I_m$ | 21.62 mA/cm$^2$ |
| Fill factor FF | 65.03 % |
| Efficiency ŋ | 13.67 % |

### 1.2.The effect of temperature on fill factor and efficiency :

Numerical modeling can be a useful tool for understanding solar and provide additional suggestions for modifying structure and cell parameters to increase cell performance. In a solar cell model, there are more than 50 parameters that can be changed [2].

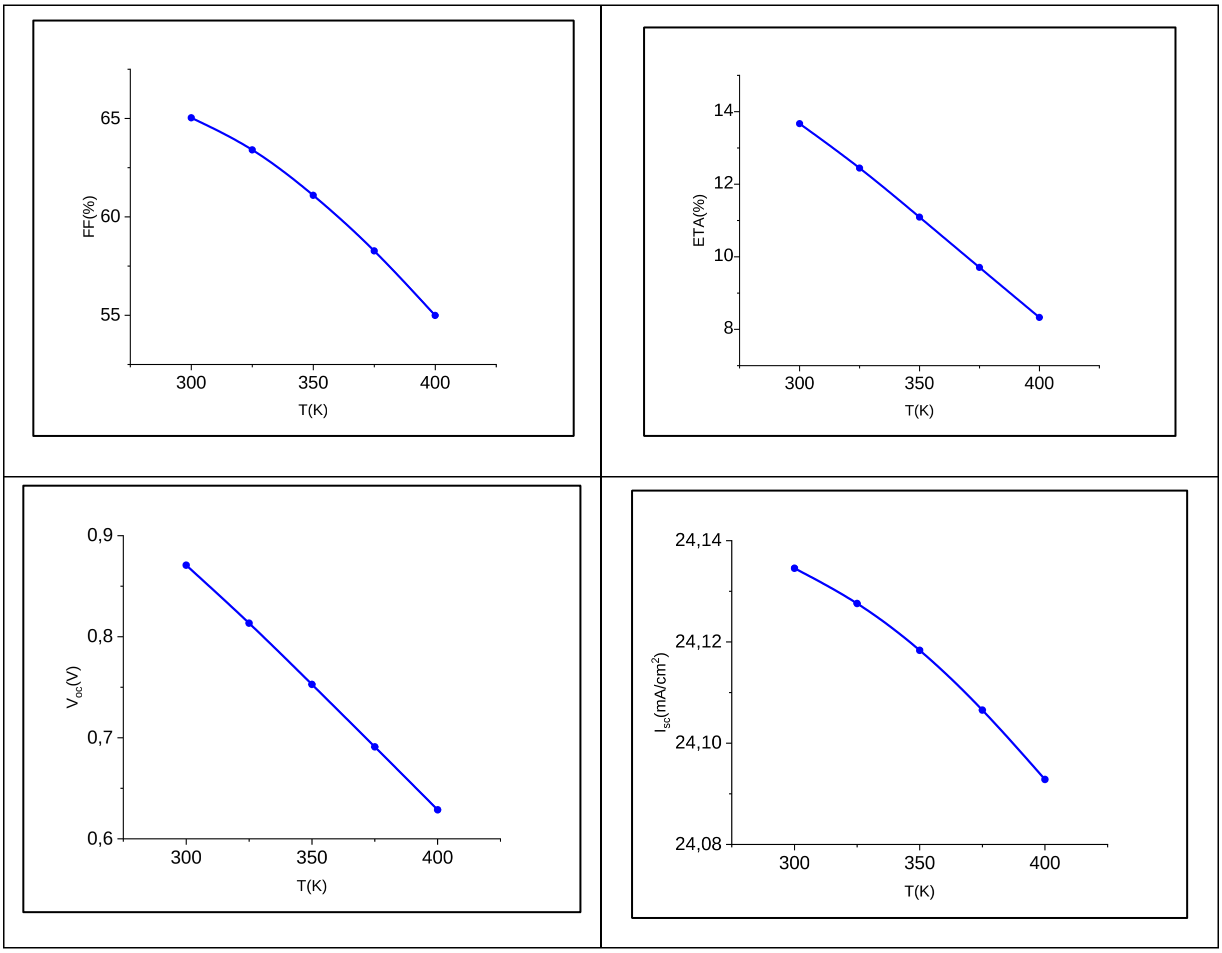



Figure 4 : The effect of temperature on $CdTe/CdS/SnO_2$ solar cell characteristics

The effect of temperature on efficiency and fill factor was studied. The results are summarized in figure 4. The temperature ranges from 300 K to 400 K.

As shown in Figure 4, we note that at 300 K we get the highest efficiency (13.66%) and fill factor is (65.03%).

While at 400 K we have the lowest efficiency (8.32%) and a fill factor of (54.99%). we note that efficiency and FF decrease when temperature increases.

From the results, the efficiency and FF are negatively affected by an increase in temperature because an increase in temperature leads to a decrease in the efficiency.

### 1.3. The effect of CdTe thickness on CdTe/CdS/$SnO_2$ solar cell characteristics :

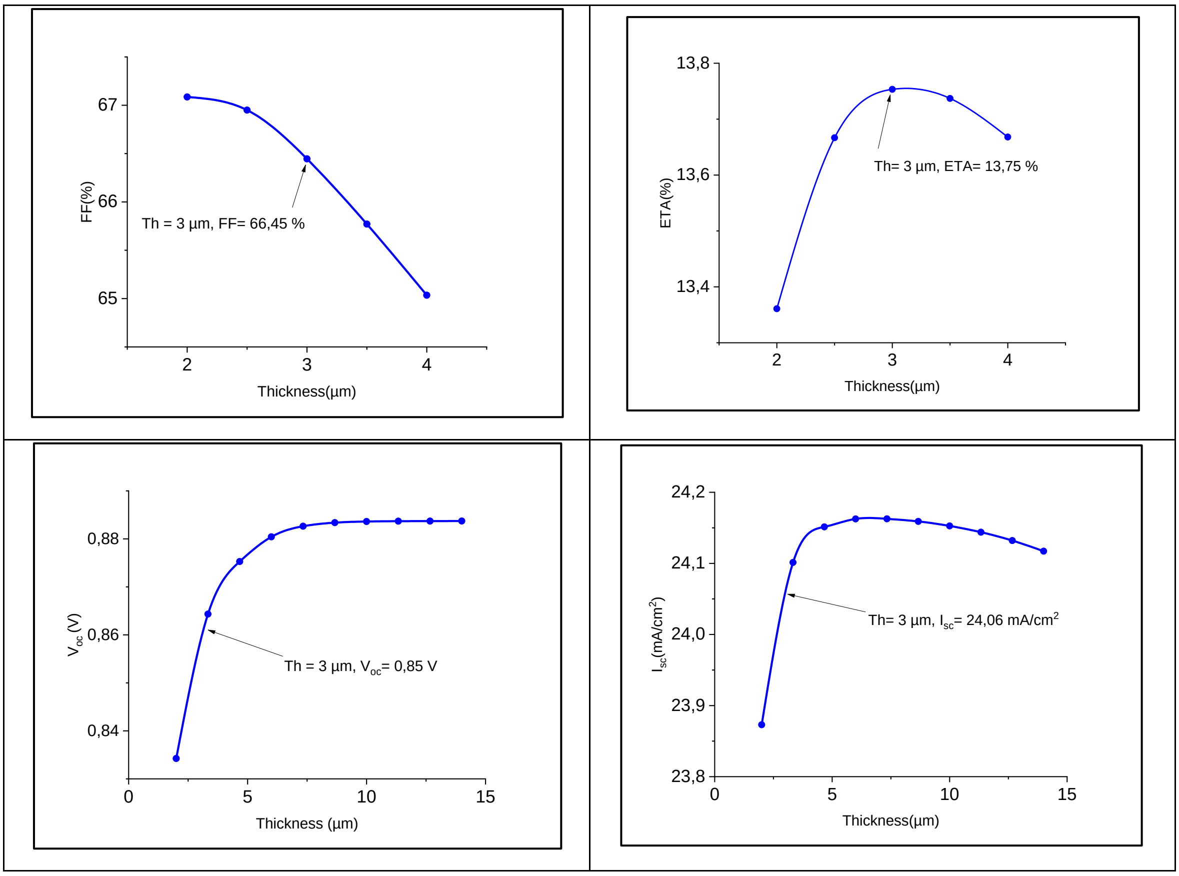



Figure 5 : Thickness vs CdTe/CdS/$SnO_2$ solar cell characteristics

We already know that a thin absorber layer correlates to poor photocurrent performance and efficiency. Furthermore, an excessively thick absorbing layer causes a significant series of resistance and an increase in material consumption, resulting in a worsening in the operational characteristics of the solar cell, and therefore an increase in the cost per unit of electricity produced[3].

Figures 5 show the effect of material thickness on fill factor and efficiency , figure 5 shows that there is a slight change in the fill factor as its value changes by 2.05% when the thickness ranges from 2 to 4 µm. A maximum value of the fill factor was obtained at 2µm.

For the solar cell in figure 6 there is also a slight change in the efficiency as it increased in the field [2 µm-3 µm] and decreased slightly in the field [3 µm-4 µm] , the highest value of the efficiency was(13.75%) at 3 µm.

From the results shown in Figure 5, we show that the thickness is inversely proportional to the increasing of the Fill Factor. The efficiency of the solar cell increases when the thickness increases until a maximum value for the efficiency at a thickness of 3 μm, then it decreases after that with thickness increasing of the absorber layer.

### 1.4. The impact of $R_s$ on $CdTe/CdS/SnO_2$ solar cell characteristics :

To study the effect of series resistance on the thin films solar cell device, a simulation was carried out by varying the series resistance from 0 to 30 $\Omega cm^2$.[4]

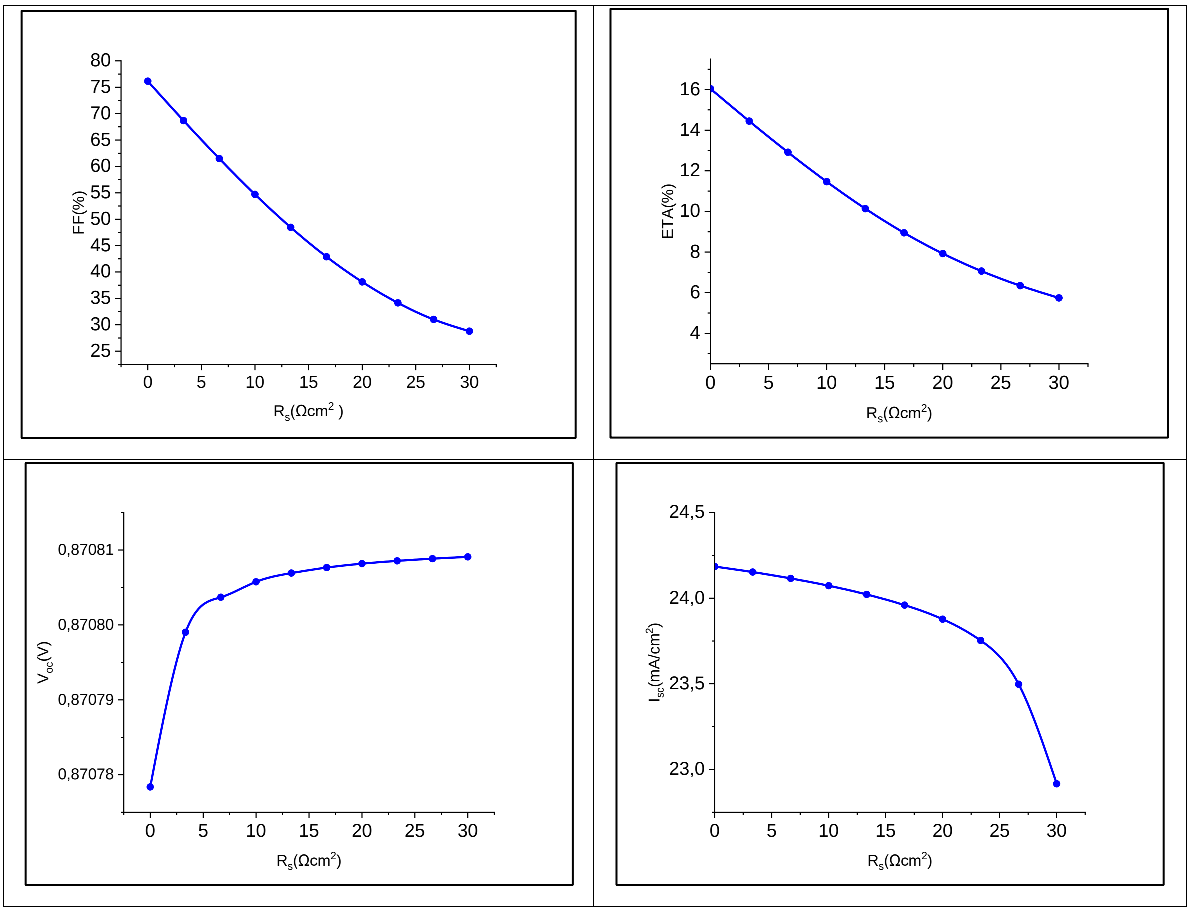



Figure 6 : Solar cell characteristics vs series resistance

From figure 6, we note that the cell efficiency, FF and $I_{sc}$ decreases with increasing of series resistance, but approximately there is no change in $V_{oc}$.

### 1.5.The impact of $R_{sh}$ on $CdTe/CdS/SnO_2$ solar cell characteristics :

Shunt resistance refers to power losses due to the recombination of electrons and holes via alternate pathways. In order to determine how the solar cell's performance would change if the shunt resistance increases from 1000 to 10000 $\Omega cm^2$ , the device was simulated.[4]

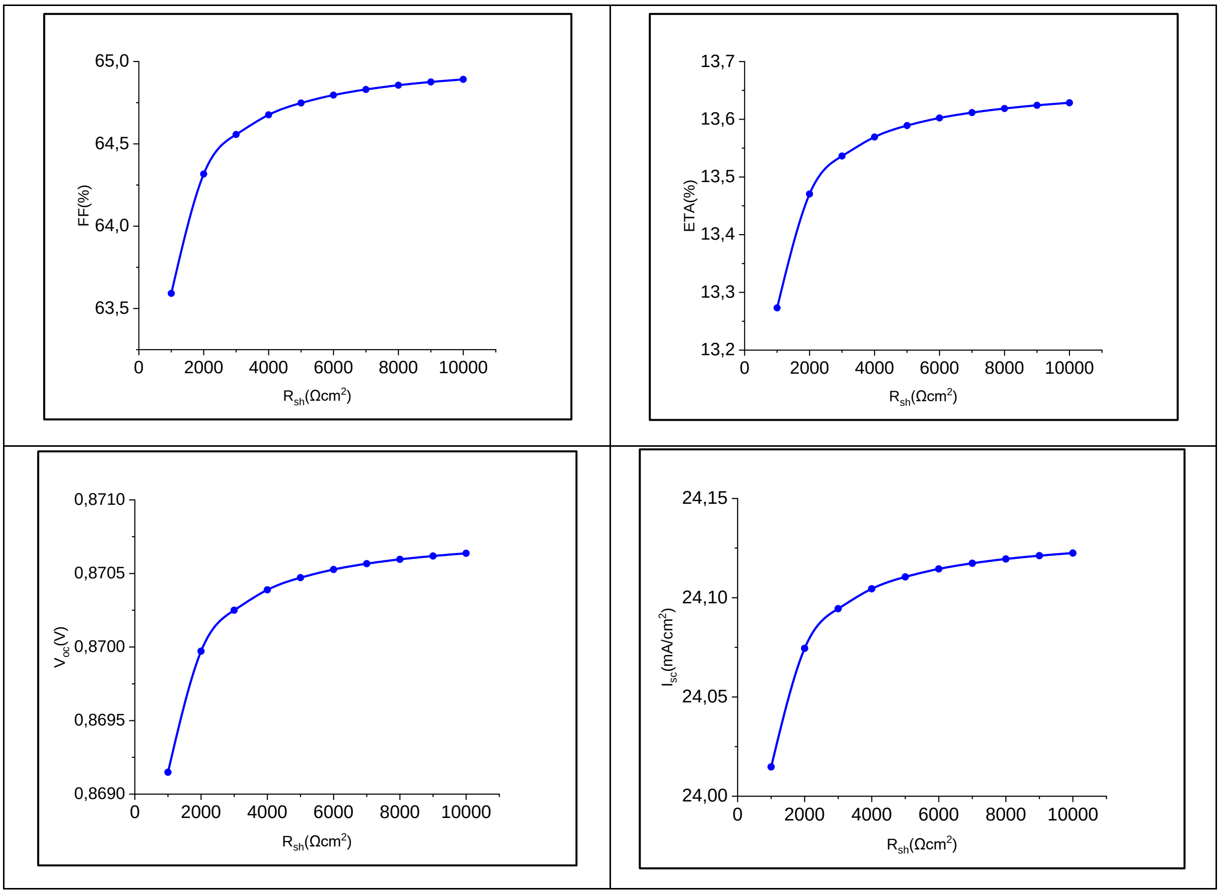



Figure 7 : $CdTe/CdS/SnO_2$ solar cell characteristics vs shunt resistance

From figure 7, the effect of the shunt resistance on the characteristics of the $CdTe/CdS/SnO_2$ solar cell is negligible. We show that the efficiency remains almost constant when the shunt resistance increases.

### 1.6.The impact of type of the absorber layer (comparison between $CIGS/CdS/SnO_2$ , $CZTs/CdS/SnO_2$ , $CdTe/CdS/SnO_2$ solar cells) :

We replace the CdTe absorber layer by an another absorber layer CIGS in the same solar cell structure. We obtain results in table 3

Table 3 : A comparison between simulating results of $CIGS/CdS/SnO_2$ , $CZTs/CdS/SnO_2$ , $CdTe/CdS/SnO_2$ solar cells

| | Simulation with CIGS absorber layer | Simulation with CZTS absorber layer | Simulation with CdTe absorber layer |
|---|---|---|---|
| $V_{oc}$ (V) | 0.49 | 0.73 | 0.87 |
| $I_{sc}$ ($mA/cm^2$) | 21.29 | 18.97 | 24.13 |
| FF (%) | 54.24 | 62.18 | 65.03 |
| ETA (%) | 5.69 | 8.65 | 13.67 |

From results shown in table 3 , Result of simulating of CdTe/CdS/$SnO_2$ with CdTe absorber layer is better than the results of CIGS/CdS/$SnO_2$ simulating with CIGS and CZTS/CdS/$SnO_2$ with CZTS absorber layer. After changing to CIGS absorber layer the efficiency decrease approximately 8% and fill factor decrease about 10%. For $V_{oc}$ the result is approximately the half of results of simulating with CdTe absorber layer.

## 2. A comparison between two solar cells simulated with SCAPS-1D :

In this part, we are going to compare between two solar cells. (a) It consists ITO as window layer, CdS as buffer layer, CdTe as absorber layer and Au as back contact layer. (b) it consists ITO as window layer, CdS as buffer layer, CZTS as absorber layer and Mo as back contact layer.

Table 4 : Metal work function of back contact for the two studied structures

| | |
|---|---|
| Work function of back metal (Au) contact layer (ev) | 5.37 |
| Work function of back metal (Mo) contact layer (ev) | 4.95 |

| | |
|---|---|
| ITO | ITO |
| CdS | CdS |
| CdTe | CZTS |
| Au | Mo |
| (a) | (b) |

Figure 8 : (a) Structure of CdTe solar cell, (b) Structure of CZTS solar cell

Table 5 : Properties of solar cells

| **Properties** | **CdTe** [5] | **CZTS** [6] | **CdS** [6] | **ITO** [7] |
|---|---|---|---|---|
| **Thickness (µm)** | 3.000 | 2.000 | 0.050 | 0.060 |
| **Band gap (eV)** | 1.500 | 1.500 | 2.420 | 3.600 |
| **Electron affinity (eV)** | 3.900 | 4.300 | 4.500 | 4.200 |
| **Dielectric permittivity (relative)** | 9.400 | 10.000 | 9.000 | 10.000 |
| **CB (1/cm^3)** | 8.000E+17 | 2.200E+18 | 1.800E+18 | 2.200E+18 |
| **VB (1/cm^3)** | 1.800E+19 | 1.800E+19 | 2.400E+18 | 1.800E+19 |
| **Electron thermal velocity (cm/s)** | 1.000E+7 | 1.000E+7 | 1.000E+7 | 1.000E+7 |

| | | | | |
|---|---|---|---|---|
| **Hole thermal velocity (cm/s)** | 1.000E+7 | 1.000E+7 | 1.000E+7 | 1.000E+7 |
| **Electron mobility (cm²/Vs)** | 3.200E+2 | 1.000E+2 | 1.600E+2 | 1.000E+2 |
| **Hole mobility (cm²/Vs)** | 4.000E+1 | 3.500E+1 | 5.000E+1 | 1.000E+1 |
| **Shallow uniform donor density ND ($cm^{-3}$)** | 0.000E+0 | 0.000E+0 | 1.000E+17 | 1.000E+19 |
| **Shallow uniform acceptor density NA ($cm^{-3}$)** | 2.000E+14 | 5.000E+16 | 0.000E+0 | 0.000E+0 |

### 2.1.A comparison between electrical characteristics :

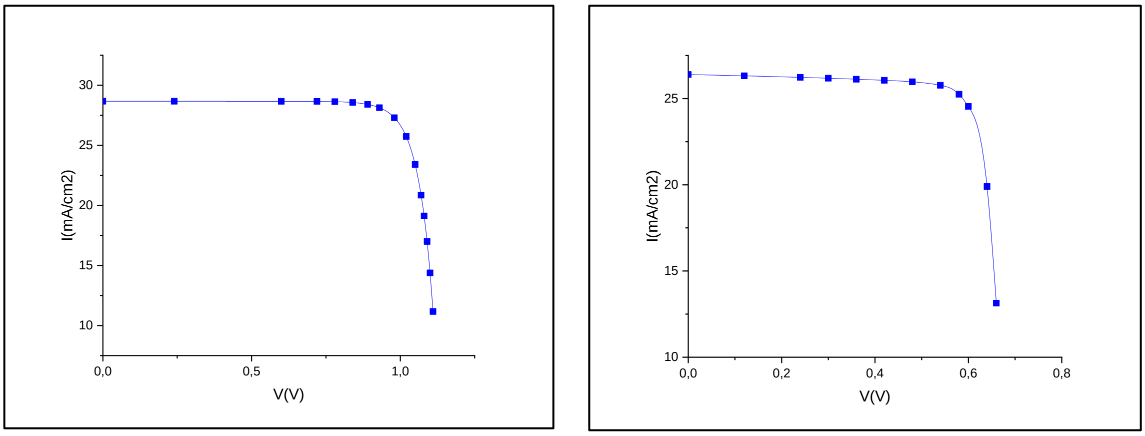
After simulating the cell (a) and (b) we obtained this characteristics :

Table 6 : Characteristics obtained from simulation

| | (a) | (b) |
|---|---|---|
| $V_{oc}$ (V) | 1.13 | 0.68 |
| $I_{sc}$ (mA/cm2) | 28.67 | 26.40 |
| FF (%) | 82.30 | 82.39 |
| ETA (%) | 26.76 | 14.76 |

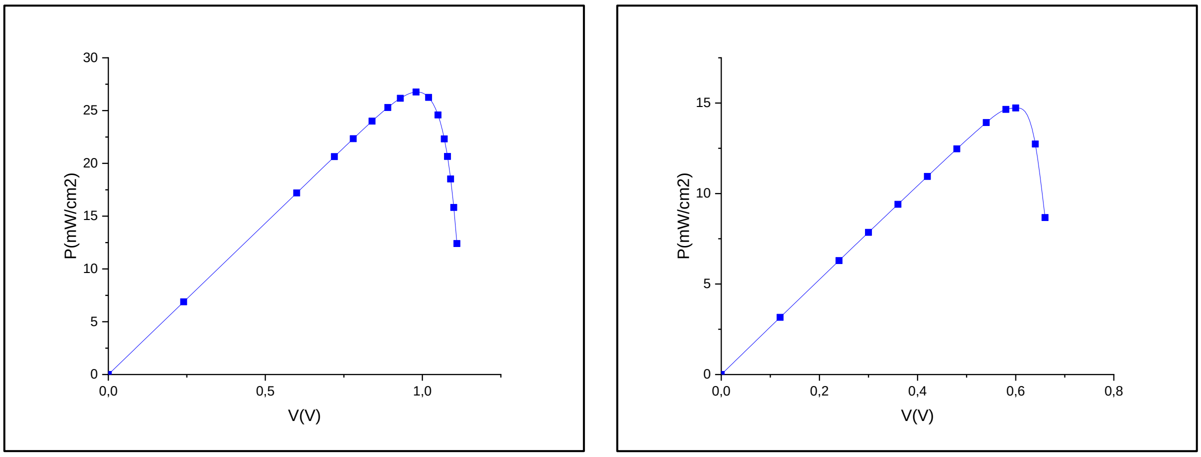
Table 6 show the results of simulating two solar cells with different absorber material. Voc ,Isc and FF have approximately the same results except the efficiency. The solar cell with CdTe absorber have higher efficiency than the solar cell with CZTS absorber there is a difference of 12%.

## 2.2.I-V and P-V curves :




(a) (b)

Figure 9 : I-V curves obtained from simulation

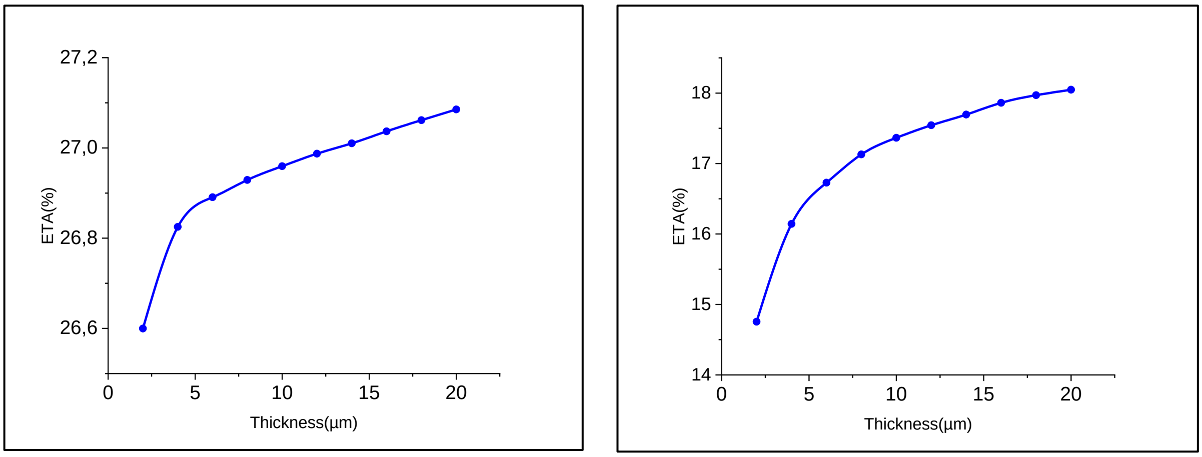



(a) (b)

Figure 10 : P-V curves obtained from simulation

From the results shown in figure 9 and 10, the influence of voltage on current and power react approximately at the same manner.

### 2.3.The effect of thickness on the efficiency :




(a) (b)

Figure 11 : Influence of thickness on the efficiency

Figure 11 show that thickness have a positive effect on efficiency even though the absorber layer is not the same.

### 2.4.The effect of ITO layer on solar cell characteristics :

Table 7 show the result of simulation solar cell without ITO layer

Table 7 : Solar cell characteristics results of simulating without ITO layer

| | (a) | (b) |
|---|---|---|
| $V_{oc}$ (V) | 1.13 | 0.68 |
| $I_{sc}$ (mA/cm2) | 28.51 | 26.37 |
| FF (%) | 80.00 | 82.14 |
| ETA (%) | 25.82 | 14.70 |

From results shown in table 7, ITO layer have no impact in $V_{oc}$ and $I_{sc}$ . for efficiency and fill factor there is a slight change on results, where simulating with ITO is better than simulating without ITO layer.

## 3. A comparison between SCAPS and with AFORS-HET simulation of Al/ZnO : Al/ZnO/CdS/CIGS/Mo solar cell :

In general, the cell consists of a thin buffer layer CdS deposited on a CIGS as an absorbent layer and a zinc oxide layer ZnO inserted between the CdS and ZnO: Al layer, and the front contact is made of Al to prevent current leakage. The back contact is Mo.[8]

Figure 12, shows the structure of simulated solar cell. The key structure sections are the CIGS absorber layer. Table 9. Gives all parameters used for the solar cell structure Using these parameters, the solar cell was simulated to get the best efficiency.

Table 8 : Metal work function for back and front contact

| | |
|---|---|
| Work function of front metal (Al) contact layer (ev) | 4.40 |
| Work function of back metal (Mo) contact layer (ev) | 4.95 |

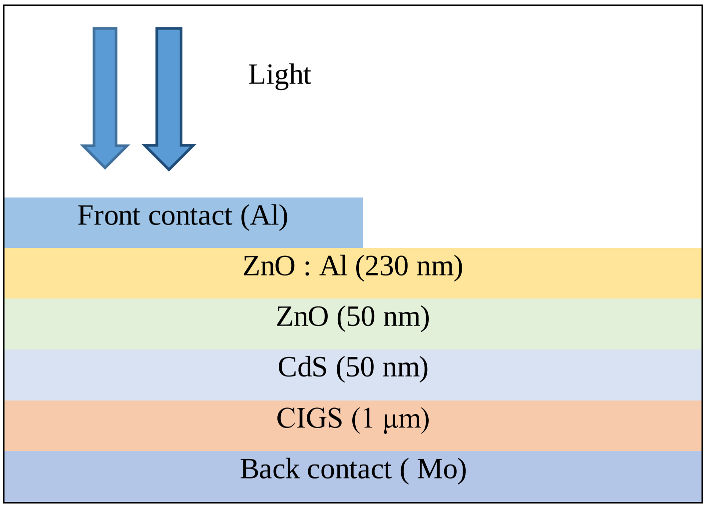



Figure 12 : Solar cell structure studied in part 2

Table 9 : Paramaters of Al/ZnO :Al/ZnO/CdS/CIGS/Mo solar cell studied

| Properties | CIGS | ZnO :Al | ZnO | CdS |
|---|---|---|---|---|
| **Thickness (µm)** | 1.000 | 0. 230 | 0.050 | 0.050 |
| **Bandgap (eV)** | 1.300 | 3.300 | 3.300 | 2.420 |
| **Electron affinity (eV)** | 4.400 | 4.500 | 4.600 | 4.200 |
| **Dielectric permittivity (relative)** | 13.600 | 9.000 | 9.000 | 10.000 |
| **CB ($cm^{-3}$)** | 2.200E+18 | 3.000E+18 | 2.200E+18 | 1.300E+18 |

| | | | | |
|---|---|---|---|---|
| **VB (cm$^{-3}$)** | 1.500E+19 | 1.800E+18 | 1.900E+19 | 9.100E+19 |
| **Electron thermal velocity (cm/s)** | 1.000E+7 | 1.000E+7 | 1.000E+7 | 1.000E+7 |
| **Hole thermal velocity (cm/s)** | 1.000E+7 | 1.000E+7 | 1.000E+7 | 1.000E+7 |
| **Electron mobility (cm²/Vs)** | 1.000E+2 | 1.000E+2 | 1.000E+2 | 7.200E+1 |
| **Hole mobility (cm²/Vs)** | 2.500E+1 | 2.500E+1 | 2.500E+1 | 2.000E+1 |
| **Shallow uniform donor density ND (cm$^{-3}$)** | 0.000E+0 | 1.000E+20 | 1.000E+18 | 1.000E+18 |
| **Shallow uniform acceptor density NA (cm$^{-3}$)** | 5.000E+15 | 0.000E+0 | 0.000E+0 | 0.000E+0 |

### 3.1.A comparison between SCAPS and AFORS-HET results :

After simulating of Al/ZnO :Al/ZnO/CdS/CIGS/Mo solar cell with SCAPS and comparison with AFORS-HET we obtain parameters in table 10:

Table 10 : A comparison between results of simulation between SCAPS and AFORS-HET

| | Simulation with SCAPS (this work) | Experimental Results[9] | Simulation with AFORS-HET [8] |
|---|---|---|---|
| $V_{oc}$ (V) | 0.44 | 0.45 | 0.45 |
| $I_{sc}$ (mA/cm$^2$) | 33.18 | 32.16 | 32.3 |
| FF (%) | 75.63 | 66.32 | 63.31 |
| ETA (%) | 11.04 | 9.65 | 9.28 |

Solar cell characteristics are obtained using SCAPS and AFORS-HET simulation are close. The efficiency is changed by 1.76% , the fill factor is increased from 63.31% to 75.63% and there is a slightly change in $V_{oc}$ and $I_{sc}$.

From the results shown, the simulation results using SCAPS program are consistent with the simulation results using AFORS-HET program for $V_{oc}$ and $I_{sc}$ , and slight change for FF and efficiency. AFORS-HET results are more close to experimental results.

### 3.2.A comparison of the effect of thickness on solar cell characteristics :

We change the CIGS thickness from 500 nm to 20 µm. We get the curve shown in figure 13 :

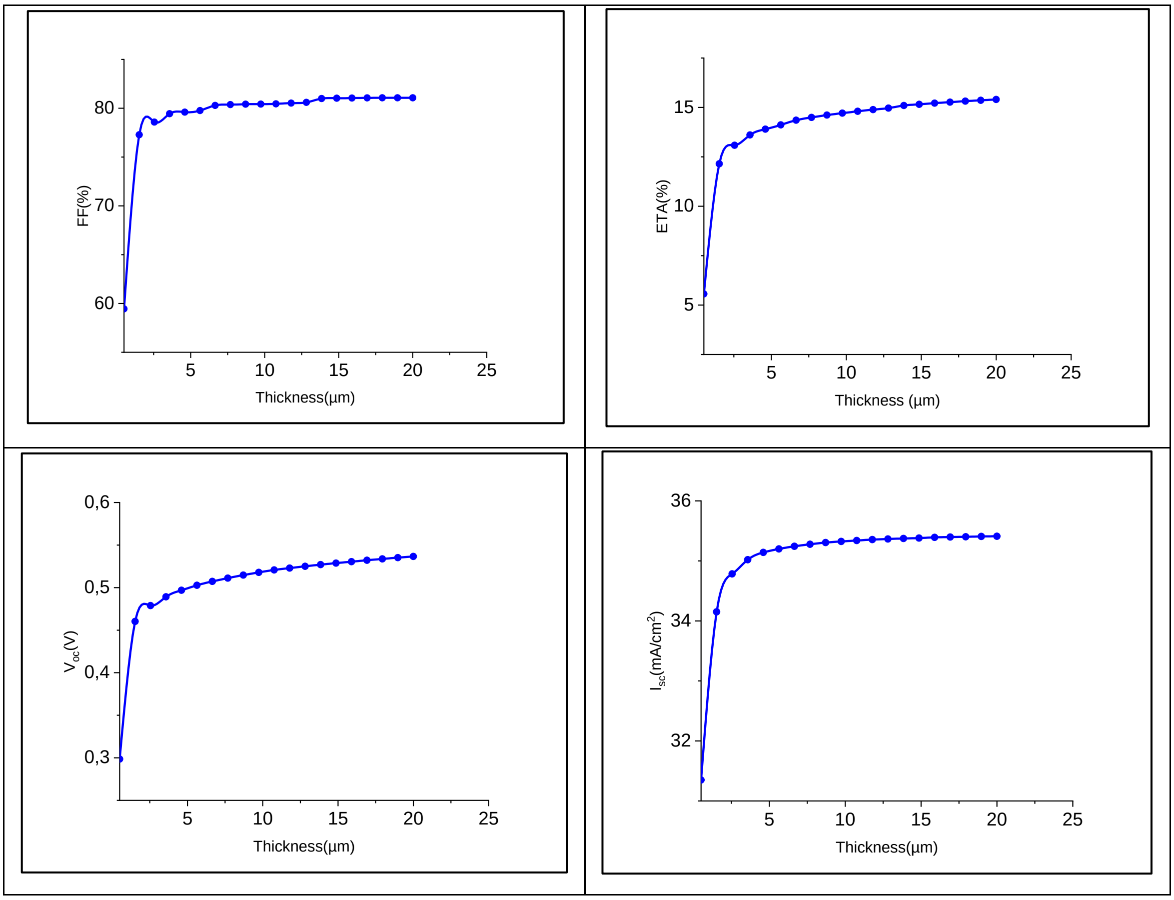



Figure 13 : Thickness vs solar cell characteristics

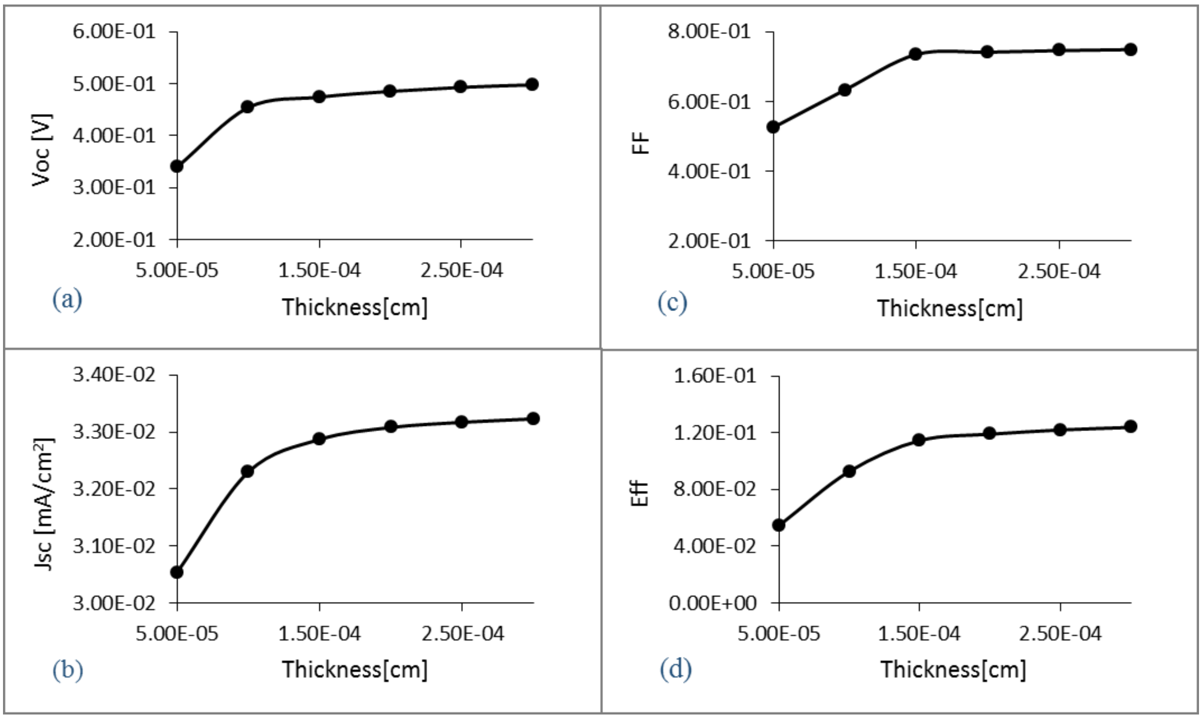



Figure 14 : The impact of thickness on solar cell characteristics ( AFORS-HET results)

Figure 13 and 14 , shows that the curves change in the same manner with the difference in the beginning of the change, and this is due to the change in the results of the properties obtained before.

### 3.3.The effect of $R_s$ and $R_{sh}$ on the efficiency :

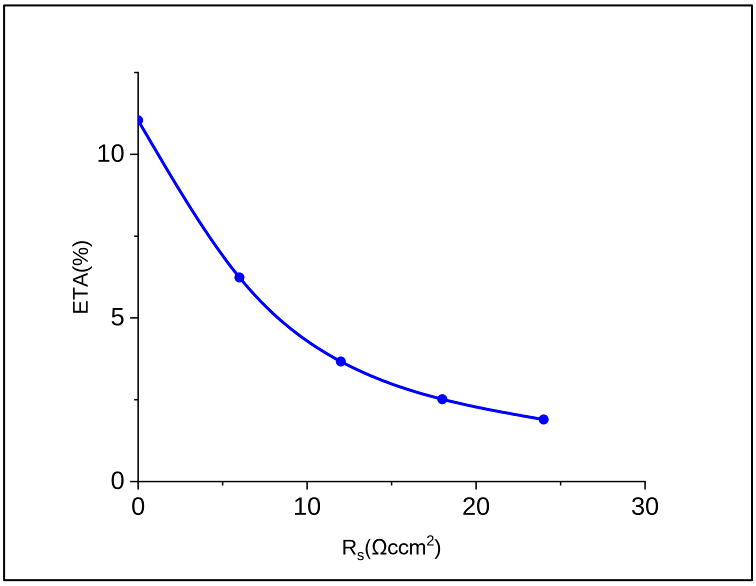



Figure 15 : Influence of $R_s$ on the efficiency

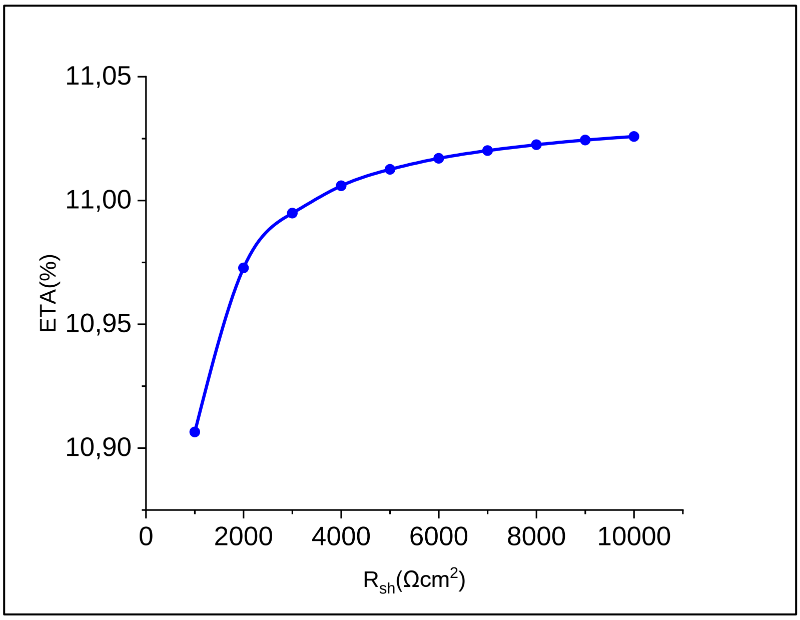



Figure 16 : Influence of $R_{sh}$ on the efficiency

From the results shown in figure 15 and 16 , the efficiency decreases slowly until it is non existent when series resistance $R_s$ =30 $\Omega cm^2$, shunt resistance have an almost non-existent impact on the efficiency.

### 3.4.The impact of type of the absorber layer :

We chaneg the absorber layer of the same structure from CIGS to CdTe, the parameters of CdTe absorber layer is shown in table 1 in the first part.

Table 11 : A comparison of simulating results of CdTe and CIGS absorber layer (part3)

| | Simulation with CIGS absorber layer | Simulation with CZTS absorber layer | Simulation with CdTe absorber layer |
|---|---|---|---|
| $V_{oc}$ (V) | 0.44 | 0.68 | 0.86 |
| $I_{sc}$ (mA/cm$^2$) | 33.18 | 26.57 | 28.50 |
| FF (%) | 75.63 | 83.00 | 84.69 |
| ETA (%) | 11.04 | 14.95 | 20.67 |

From results shown in table 7 , Result of simulating with CdTe absorber layer is better than the results of simulating with CIGS and CZTS absorber layer of this structure. After changing too CIGS absorber layer the efficiency and fill factor decrease approximately about 10%. For

$V_{oc}$ the result is approximately the half of results of simulating with CdTe absorber layer, and $I_{sc}$ increase about 5 mA/cm$^2$.

## Conclusion

From results shown in this chapter, different structures react with different manners. First, thickness have a positive effect on efficiency until a specific value that change according to the type of absorber layer and the solar cell structure after that it will effect the efficiency negatively. Next, series resistance have a negative effect on efficiency while shunt resistance do not have any impact and the type of absorber layer make an impact as well , we found that CdTe absorber layer have the best efficiency for the studied solar cells. Finally, adding ITO layer have a slightly positive impact on efficiency and fill factor.

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# General conclusion

# General conclusion

Solar cells has been always the easiest way to convert solar energy to electricity. To keep up with times , solar cell is been developed and use nanotechnology. Due to the hardest way to do experiments in thin film solar cells , it is simulated through various programs such as SCAPS-1D, AFORS-HET, SILVACO-ATLAS, AMPS and more others. SCAPS-1D is the most usable and suitable software for the photovoltaic conversion of semiconductor devices.

In this work, we started with generalities of solar cells such as, types working principals, how solar cells are simulated and more other information.

Next, we got to know SCAPS-1D simulation program , how this program works and how to obtain results. Finally we started simulating solar cells using this program.

This simulation allowed us to study the effect of different parameters on solar cell characteristics. The analysis of all of our results shows that :

1. Temperature have a negative effect on the efficiency of solar cells , the lowest temperature which is 300K causes the highest efficiency and same for $V_{oc}$ , $I_{sc}$ and FF .
2. Series resistance have a negative effect on efficiency, FF and $I_{sc}$ while the $V_{oc}$ increase by the increase of resistance . Series resistance become approximately not existed after 25 $\Omega cm^2$.
3. Shunt resistance have approximately no effect on the characteristics of solar cells, but it is better to select shunt resistance of 6000 $\Omega cm^2$.
4. Thickness effect in different ways due to different structures. For the first studied structure, it effect positively on efficiency , $V_{oc}$ and $I_{sc}$ until 3μm after that she effect negatively. For the second and the third studied structure , it effect just positively in the field studied and the efficiency begin to stabilized at the same previous value.
5. We compared between the results of three different absorber layers (CdTe , CIGS and CZTS) , we found that absorber layer from CdTe type have the best results.
6. We compared between results simulated with SCAPS-1D and results of AFORS-HET, we found that the results of SCAPS-1D is better than the results of AFORS-HET. But the results of AFORS-HET is closer to the experimental results.

7. We compared between two structures simulated with SCAPS-1D, we found that the results of ITO/CdS/CdTe/Au structure are better than the results of ITO/CdS/CZTS/Mo structure.
8. We compared between results of the presence of ITO layer and the absence of it , we found that ITO have a slightly positive impact on the efficiency , FF, $V_{oc}$ and $I_{sc}$

**Abstract:** This study aims to simulate thin-film solar cells using the SCAPS-1D program. The cell with CdTe/CdS/SnOx structure was studied. We obtained the characteristics of the cell and found that the current-voltage curve and the power curve correspond to the theoretical curves of solar cells. We studied the effect of temperature on the filling modulus and cell yield. Simulation results showed that high temperature negatively affects the filling coefficient and cell efficiency. We found that the thickness of e = 3 mm for the CdTe layer in the studied cell gives the best yield for it. Its highest efficiency was at T=300K , η =13.75% the packing plant estimated at that time FF = 66.45%, while the short circuit current was estimated at $I_{sc}$ = 24.06 mA/cm2. The open circuit voltage under these conditions is rated $V_{oc}$ = 0.85 V The study showed that increasing the series resistance negatively affects the work of the studied cell, as the packing coefficient and its efficiency are almost non-existent when the series resistance is greater than 25 Ωcm2. Increasing series resistance negatively affects $I_{sc}$ but does not affect $V_{oc}$. We found that the effect of parallel resistance on solar cell properties is almost negligible. In order to study the effect of the absorbent layer on the efficiency of the solar cell, we compared three cells: $CIGS/CdS/SnO_x$, $CZTS/CdS/SnO_x$, and $CdTe/CdS/SnO_x$. We also compared the two cells ITO/CdS/CdTe/Au and ITO/ CdS/CZTS/Mo The results showed that the CdTe absorbent layer solar cell is the best. We conducted a study of the Al/ZnO /ZnO/CdS/CIGS/Mo cell in order to compare our results with the results obtained from another reference. Our results were in agreement with the experimental results and simulation results using the AFORS-HET program.
Keywords: solar cells, thickness, series and shunt resistance, SCAPS-1D, ITO, CdTe.

**Résumé :**Cette étude vise à simuler des cellules solaires à couches minces à l'aide du programme SCAPS-1D. La cellule à structure $CdTe/CdS/SnO_2$ a été étudiée. Nous avons obtenu les caractéristiques de la cellule et constaté que la courbe courant-tension et la courbe de puissance correspondent aux courbes théoriques des cellules solaires. Nous avons étudié l'effet de la température sur le module de remplissage et le rendement cellulaire. Les résultats de la simulation ont montré qu'une température élevée affecte négativement le coefficient de remplissage et l'efficacité de la cellule. Nous avons constaté que l'épaisseur de e = 3 mm pour la couche de CdTe dans la cellule étudiée donne le meilleur rendement pour celle-ci. Son rendement le plus élevé était à T=300K , η =13,75% l'usine de conditionnement estimait alors FF = 66,45%, tandis que le courant de court-circuit était estimé à $I_{sc}$ = 24,06 mA/cm2. La tension en circuit ouvert dans ces conditions est notée $V_{oc}$ = 0,85 V L'étude a montré que l'augmentation de la résistance série affecte négativement le travail de la cellule étudiée, car le coefficient de compactage et son efficacité sont quasi inexistants lorsque la résistance série est supérieure à 25 Ωcm2. L'augmentation de la résistance série affecte négativement $I_{sc}$ mais n'affecte pas $V_{oc}$. Nous avons constaté que l'effet de la résistance parallèle sur les propriétés des cellules solaires est presque négligeable. Afin d'étudier l'effet de la couche absorbante sur l'efficacité de la cellule solaire, nous avons comparé trois cellules : $CIGS/CdS/SnO_2$, $CZTS/CdS/SnO_2$ et $CdTe/CdS/SnO_2$. Nous avons également comparé les deux cellules ITO/CdS/CdTe/Au et ITO/CdS/CZTS/Mo. Les résultats ont montré que la cellule solaire à couche absorbante CdTe est la meilleure. Nous avons mené une étude de la cellule Al/ZnO/ZnO/CdS/CIGS/Mo afin de comparer nos résultats avec les résultats obtenus à partir d'une autre référence. Nos résultats étaient en accord avec les résultats expérimentaux et les résultats de simulation à l'aide du programme AFORS-HET.
Mots clés : cellules solaires, épaisseur, résistance série et shunt, SCAPS-1D, ITO, CdTe.

**ملخص**: تهدف هذه الدراسة الى محاكاة خلايا شمسية ذات الأغشية الرقيقة باستعمال برنامج SCAPS-1D. تمت دراسة الخلية ذات البنية $CdTe/CdS/SnO_2$. تحصلنا على خصائص الخلية و وجدنا أن منحنى تيار جهد و منحنى الاستطاعة يتوافقان مع شكل المنحنيات النظرية للخلايا الشمسية. درسنا تأثير درجة الحرارة على معامل التعبئة و مردود الخلية. بينت نتائج المحاكاة أن ارتفاع درجة الحرارة يؤثر سلبا على معامل التعبئة و كفاءة الخلية. وجدنا أن سمك e = 3µm للطبقة CdTe في الخلية المدروسة يعطي أفضل مردود لها. كانت أعلى كفاءة لها عند T= 300 K هي η = 13,75% يقدر معمل التعبئة عندئذ ب FF=66,45 % أما تيار دارة القصر فيقدر ب $I_{sc}$ = 24,06 $mA/cm^2$. يقدر جهد الدارة المفتوحة في هذه الظروف ب $V_{oc}$ = 0,85 V. بينت الدراسة أن زيادة المقاومة التسلسلية يؤثر سلبا على عمل الخلية المدروسة حيث أن معامل التعبئة و كفاءتها تنعدم تقريبا عند مقاومة تسلسلية أكبر من 25 $\Omega cm^2$. يؤثر تزايد المقاومة التسلسلية سلبا على $I_{sc}$ لكنه لا يؤثر على $V_{oc}$. وجدنا أن تأثير المقاومة التفرعية على خصائص الخلية الشمسية مهمل تقريبا. من أجل دراسة تأثير الطبقة الماصة على كفاءة الخلية الشمسية, قمنا بالمقارنة بين ثلاث خلايا هي $CIGS/CdS/SnO_2$, $CZTS/CdS/SnO_2$, و $CdTe/CdS/SnO_2$. أجرينا كذلك مقارنة بين الخليتين ITO/CdS/CdTe/Au و ITO/CdS/CZTS/Mo أظهرت النتائج أن الخلية الشمسية ذات الطبقة الماصة CdTe هي الأفضل. قمنا باجراء دراسة للخلية Al/ZnO /ZnO/CdS/CIGS/Mo من أجل المقارنة بين نتائجنا و النتائج المتحصل عليها من مرجع أخر. كانت نتائجنا على توافق مع النتائج التجريبية و نتائج محاكاة باستعمال برنامج AFORS –HET.
الكلمات المفتاحية : خلايا شمسية، السمك، مقاومة تسلسلية و تفرعية، SCAPS-1D، ITO، CdTe