

**EFFECT OF TiO₂ ON THE PERFORMANCE OF DYE SENSITIZED SOLAR
CELL (DSSC) SIMULATED USING ATLAS**

By

NURUL ATIQAH BINTI MOHD SARGAWI

FINAL PROJECT REPORT

Submitted to the Department of Electrical & Electronic Engineering
in Partial Fulfillment of the Requirements
for the Degree
Bachelor of Engineering (Hons)
(Electrical & Electronic Engineering)

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CERTIFICATION OF APPROVAL

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Nurul Atiqah bt Mohd Sargawi

A project dissertation submitted to the
Department of Electrical & Electronic Engineering
Universiti Teknologi PETRONAS
in partial fulfilment of the requirement for the
Bachelor of Engineering (Hons)
(Electrical & Electronic Engineering)

Approved:

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Project Supervisor

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May 2012

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

Nurul Atiqah Bt Mohd Sargawi

ABSTRACT

Dye-Sensitized Solar Cell (DSSC) has gained much interest due to its low cost of fabrication. Many researches have been carried out to optimize its properties and structure for maximum efficiency and fill factor. In this paper, predicting the efficiency of a DSSC for optimization purposes using Silvaco ATLAS is outlined. Initially, DSSCs with TiO_2 /dye absorption layer thickness of 6 μm , 12 μm and 18 μm were fabricated. The absorbance of each layer was then measured using UV-Vis. From the absorbance data, the reflection and refraction coefficients were calculated using Kramers Kronig equations. They were later used in ATLAS to simulate the efficiency of the DSSC. In the simulation, the DSSC was modeled as two organic sandwiched regions which consist of TiO_2 coated dye and electrolyte. AM 1.5 spectra is used as a light source. For each single photon from the light source, a singlet is assumed to be created. Singlet equation is then solved accounting for Langevin recombination and singlet exciton dissociation. The outcome from ATLAS shows that better efficiency can be achieved using 18 μm thick TiO_2 /dye absorption layer. The outcome is validated by measuring the actual efficiency of the fabricated DSSC. Close agreement between the predicted and measured efficiency suggest that ATLAS can be used as a tool to optimize the DSSC.

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CHAPTER 1

INTRODUCTION

1.1 Project background

Nowadays, silicon based solar cells is dominating the solar cell market. However, the main issue is the production cost that is even higher than the output power produced by it. Dye sensitized solar cell (DSSC) is anew technology of solar cell which can be made from various material. But, this type of solar cell is having issue regarding its efficiency level. Thus, many researches have been done in order to increase the performance of this DSSC.

1.2 Problem Statement

In pursuing higher efficiency of DSC, numerous researches have been done to study and understand the mechanism of DSC. Up to now, efficiency for DSSC still lower than Silicon based solar cell. So, instead of using experimental method in analyzing the DSSC performance, there is a need to identify or develop software that can analyze the efficiency of DSSC.

1.3 Objective & Scope of Study

Objectives for this study are:

- 1) To study the effect of thickness variation in TiO_2 layer toward DSSC performance.
- 2) To obtain the complex refractive index based on UV-VIS data.
- 3) To identify ATLAS ability in simulating the DSSC performance.

Scope of study:

- 1) Modeling and simulation of DSSC with varying photoelectrode thickness.
- 2) To do experiment to observe the DSSC performance experimentally with the supervision of authorized personnel.

1.4 Relevancy

This paper wants to verify the ATLAS ability in simulating the DSSC performance. if this software can accurately analyze the DSSC performance as close as the experimental value, thus this software proven reliable.

1.5 Feasibility

The feasibility of this project is to complete the project within the allocated time frame, while maintaining the consistency of this project.

During the first semester (FYP I), the scope and task that will be covered are:

- a) Researching about the DSC and specifically about TiO_2 layer.
- b) Produce paper work to propose this study.

CHAPTER 2

LITERATURE REVIEW

2.1 Solar Cell Generation

2.1.1 First Generation Solar Cells

First generation solar cell is silicon based solar cell that still dominates the solar panel market due to its high efficiency [13][14]. This type of solar cell account for 86% of the solar market due to its high endurance level compared to the other type of solar cell [13]. However, fabricating silicon based solar cell required a very high cost and they tend to lose some of their efficiency at the high temperature place like during the hot sunny day [13][14].

Currently, there four types of silicon that has been used in the solar panel production which are monocrystalline solar cells, polycrystalline solar cells, amorphous silicon solar cells and hybrid silicon solar cells.

2.1.2 Second Generation Solar Cell

Second generation solar cells are thin film based that having a cheaper production cost compared to the first generation. However, it has lower efficiencies. There three types form this generation which are amorphous silicon, cadmium telluride (CdTe), and copper indium gallium diselenide (CIGS) [14]. Both CdTe and CIGS are non-silicon materials. Second generation solar cells need less support when placing panels on rooftops, able to achieved lower cost per watt, reduce mass and the panel can be rolled out onto a roof or other surface [13][14][15].

2.1.3 Third Generation Solar Cell

Third generation solar cells are completely different from the previous one as it can be made from various materials besides silicon. This generation didn't rely on the p-n junction in order to separate photogenerated charge carriers

[13] [14] [15]. It contains a wider range for potential solar innovations such as polymer solar cells, nanocrystalline cells and dye-sensitized solar cells [14] [15]. For this project, the author studies the performance of dye sensitized solar cells (DSSC).

2.2 Dye-Sensitized Solar Cell (DSSC)

Nowadays, Silicon based solar cell is widely used with approximately 25% in efficiency. But, the weakness is the high production cost which is costly than the source of energy from fossil and also difficult to fabricate. In 1991, DSSC had been invented by Michael Grätzel and Brian O'Regan at the École Polytechnique Fédérale de Lausanne. [11-12] DSSC is an electrochemical device that generates electricity from the sunlight using the dye-molecules which are light-absorbing adsorbed on semiconductor particles.[1] DSSC contains mesoporous nanocrystalline semiconductors like TiO₂, ZnO and SnO₂ as photoanodes anchored with dye molecules which serve as light harvesters fabricated on Transparent Conducting oxide (TCO), a platinum (Pt) counter electrode and an electrolyte solution with dissolved iodide ion/ tri- iodide ion redox couples between electrodes. [6] Dye sensitizers function as light absorber and then exploit the light energy to induce vectorial electron transfer reaction. [6]

The conversion efficiency (η) of solar cell can be represented by this equation:
[6]

$$\eta = FF \times I_{SC} \times V_{OC} / P_{in}$$

Where FF is fill factor, I_{SC} is short circuit current, V_{OC} is open circuit voltage and P_{in} is incident power. This equation shows that in order to raise the conversion efficiency, these four parameters are necessary to be improved. In DSSCs, its series resistance consists of three resistance elements which are sheet resistance of TCO, the resistance of ionic diffusion in the electrolyte and the resistance at the interface between the counter electrode (CE) and the electrolyte. [6]

Due to low production cost, DSSCs are promising for more cost effective than conventional solar cells. This low production cost is because of cheap printable materials

and simple manufacturing techniques. [1] However, less efficiency of power conversion is the main issue that has been under research for past 10 years besides its shorter operating lifetime. For now, some reported that DSSC efficiency currently improved to 11.5% and the other reported it about 10% - 10.8%. [6-7, 9] However, insufficient understanding about DSC mechanism behavior caused us to rarely achieved efficiency of over 10%. [6] Present focus is to find all factors that can lead to higher energy conversion, lower cost and also longer operating lifetime. [2]

2.2.1 Basic Structure

Typical DSSC consists of transparent conductive oxide (TCO) layer, photoelectrode film (PE film) layer, electrolyte, and counter electrode layer (CE). TCO is coated with glass or plastic which is transparent and electrically conductive. Photoelectrode is nanophorous film consisting of interconnected TiO_2 particles covered with dye molecules. [1] These dye molecules absorb light from the sun and TiO_2 will provide sufficient amount of dye for efficient light absorption and also play important role by ensuring that dye molecules are in direct contact with both TiO_2 and electrolyte by functioning as electron acceptor and electronic conductor. [1, 7] This photoelectrode is only 10 μm thick. [1] Counter electrode layer is the same as TCO layer but coated with platinum catalyst particles. Figure 1 shows the structure of DSSC.

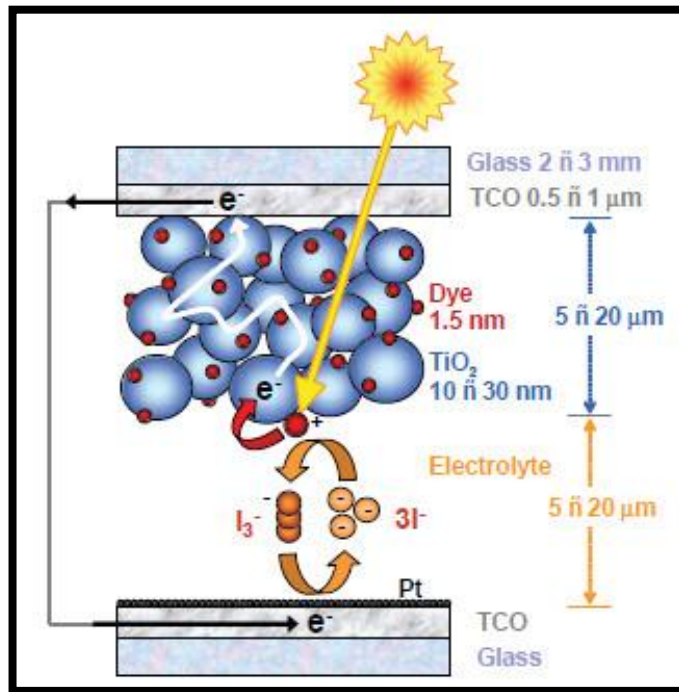


Figure 1: DSSC structure [1]

2.2.1.1 Titanium Dioxide layer

There are many photoelectrodes made from such material as Si, GaAs, and CdS. However, oxide semiconductor materials have few advantages compare to the other types. First, TiO_2 a good chemical stability when exposed under visible irradiation in solution. Second, they are cheap and nontoxic. Third, TiO_2 thin film can be prepared by only using a very simple process. TiO_2 film normally contains large TiO_2 nanoparticles which is around 250-300 nm. This TiO_2 film can be prepared by a very simple process where TiO_2 colloidal solution or paste is coated on the TCO substrate and then sintered at 450 to 500°C

2.2.1.2 Redox electrolyte

Most common electrolyte used in DSSC is I-/I₃⁻ redox ions which functions as the electron mediator between the TiO₂ photoelectrode and the counter electrode.

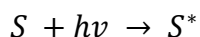
2.2.1.3 Counter electrode

Reduction of the dye cations with I⁻ ion will form the tri-iodide ion which is I₃⁻ which then will be re-reduce to I⁻ ions at the counter electrode. For the counter electrode to be able to do this task, it must have high electrocatalytic activity. Thus, platinum, Pt which which coated on TCO substrate will usually use as the counter electrode.

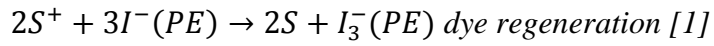
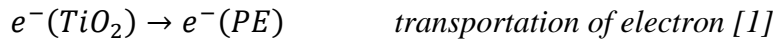
2.2.2 Operation

Basically, when the dye absorbs photon from the sunlight, electron will excited from low energy state to a higher energy state of the molecule (S⁰ to S¹). [1, 10] Next, electron will be injected to the TiO₂ band and will be transported to TCO layer. [1, 3] electron donation from the electrolyte such as iodide/tri iodide couple will restore the original state of the dye subsequently. [8] Electron captured from the redox electrolyte will regenerated the oxidized dye. The injected electron will travel by diffusion in the TiO₂ film. Electron mobility in TiO₂ is about 40 to 1 cm² s⁻¹ V⁻¹. [3] When it finds its way to substrate contact, it will be released to the external electrical circuit. Illumination that corresponds to the difference between the Fermi level of the electron solid and the redox potential of the electrolyte will generate the voltage. [8] Then, by electrolyte reduction reaction at the counter electrode, the electron is returned to the cell. The ionic transport of the redox pair in the electrolyte will complete the electrical circuit and thus generated electric power without suffering any permanent chemical transformation. [1, 8] Operating cycle can be summarized as per equation below taken from [1]:

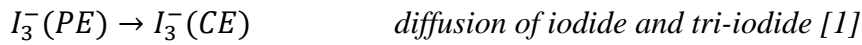
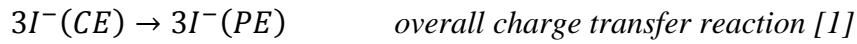
For photoelectrode:



dye absorbs the sunlight [1]



For counter electrode:



Total reactions:

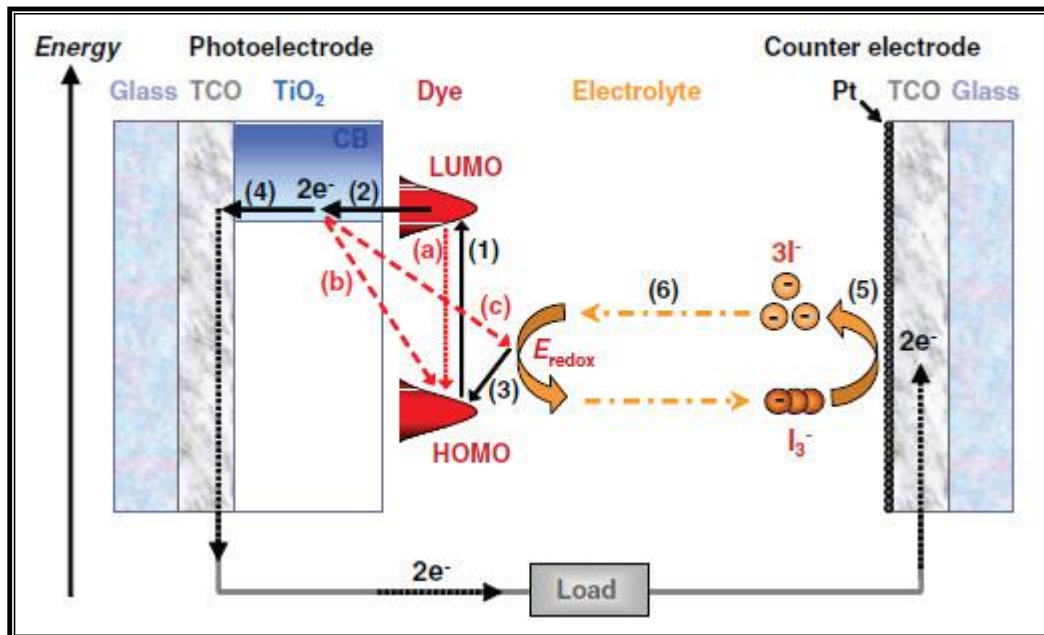
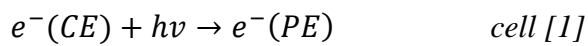
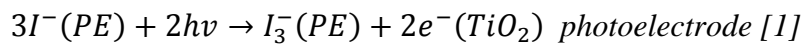


Figure 2: DSSC operation. [1]

2.3 Optical properties

Optical properties of the substances define as the changes that the light undergoes when interacting with a particular substance. There are many optical properties if we were to consider, but the most well know are reflection, refraction, transmission and absorption. Those optical properties are associated with most important optical properties like absorption coefficient, extinction coefficient and also refractive index.

2.3.1 Absorption coefficient

Absorption and absorption coefficient is closely related since absorption coefficient can be obtained using the absorption value. The definition of absorption coefficient is really important because some use the natural log while the other some use log to the base 10. When illumination of wavelength and intensity impinges on a material thickness which denotes as d , some part light will be reflected while the other part will be emerged to the other side of the material at d . These I , R and T are related by the expression below:

$$I(\lambda) = T(\lambda) + R(\lambda) + A(\lambda) \quad (1)$$

$I(\lambda)$, $T(\lambda)$, $R(\lambda)$ and $A(\lambda)$ are intensity, transmittance, reflectance and absorption taking place for this wavelength. Next, by applying the Beer-lambert law, the relationship between T and $I-R$ become

$$T(\lambda) = [I - R][1 - e^{-\alpha(\lambda)d}] \quad (2)$$

Where $\alpha(\lambda)$ is absorption coefficient at the wavelength λ . Then, the equation become

$$A(\lambda) = [I - R][1 - e^{-\alpha(\lambda)d}] \quad (3)$$

We then can rearranged the equation (2) become

$$\frac{T(\lambda)}{I(\lambda) - R(\lambda)} = e^{-\alpha(\lambda)d} \quad (4)$$

Relationship between absorbance and transmittance is,

$$A_{abs}(\lambda) = -\ln \left[\frac{T(\lambda)}{I(\lambda)-R(\lambda)} \right] \quad (5)$$

By equating equation (4) and (5), we get

$$\alpha(\lambda) = \frac{A_{abs}(\lambda)}{d} \quad (6)$$

For this project, the author used equation (6) to obtain the absorption coefficient value.

2.3.2 Refractive index and extinction coefficient

Extinction coefficient is related with the absorption coefficient by this equation:

$$\alpha = \frac{4\pi k}{\lambda} \quad (7)$$

By rearrange this equation, we get

$$k = \frac{\alpha\lambda}{4\pi} \quad (8)$$

Equation (8) had been used throughout this project to obtain the extinction coefficient or k value.

Refractive index, n of an optical medium is actually the ratio of the velocity of the light which is c in vacuum to its velocity, v in the medium, $n = c/v$. complex refractive index, denotes by N is consists of n as the real part and k as the imaginary part. In short, N can be expressed as below:

$$N = n - iK \quad (9)$$

In order to obtain the n , Kramers-Kronig relation can be used since the extinction coefficient which is the imaginary part can be calculated beforehand. This requires the value of frequency dependence of either the real or imaginary part over a wide frequency range.

The kramers-kronig relation is given by [16],

$$n(\omega) - 1 = \frac{2}{\pi} P \int_0^{\infty} \frac{\omega' K(\omega')}{\omega'^2 - \omega^2} d\omega'$$

$$K(\omega) = -\frac{2}{\pi} P \int_0^{\infty} \frac{n(\omega') - 1}{\omega'^2 - \omega^2} d\omega'$$

Where ω' the integration variable and P represents the Cauchy principal value of the integral and the singularity at $\omega = \omega'$ is avoided. n and K is the real part and the imaginary part. Since the Kramers- Kronig involved with complicated measurement, the calculation of the real part will be done using MATLAB.

CHAPTER 3

METHODOLOGY

3.1 Research Methodology

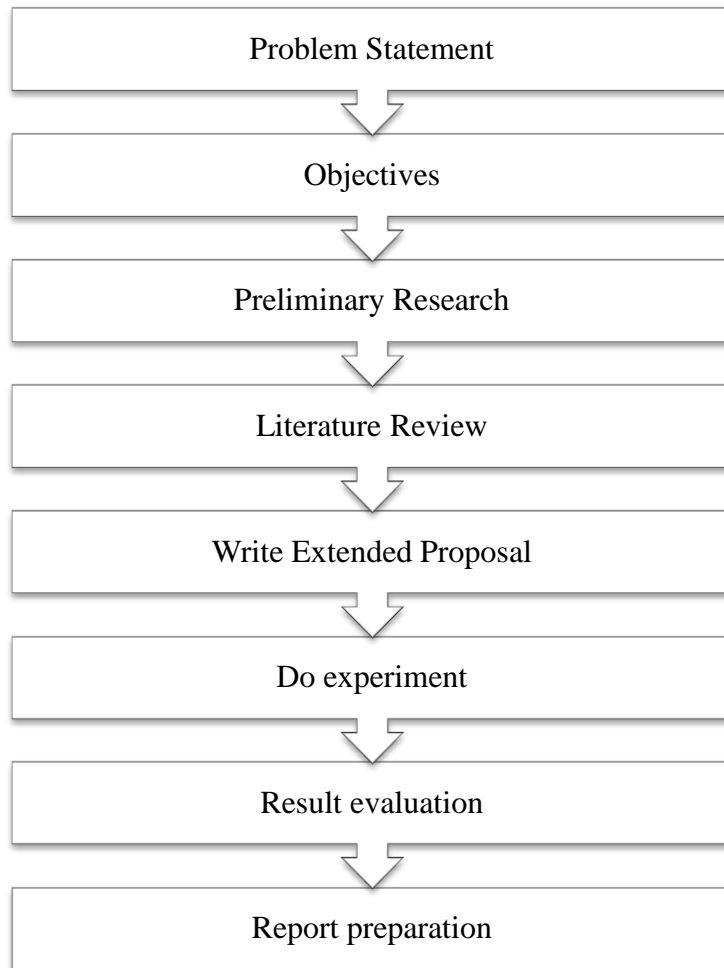


FIGURE 3: Project Methodology

3.2 Assumption

For this project, an assumption has been made to simplify the experiment and focus to only one factor which is TCO layer thickness variation which is setting n and k value to be constant where n and k is electron concentration and Boltzmann's constant.

3.3 Experiment Procedures

For the experiment procedure, the author needs to get the absorbance data for every thickness. The author uses three different thicknesses which are $6\mu\text{m}$, $12\mu\text{m}$ and $18\mu\text{m}$. These absorbance data will be obtain through UV-VIS experiment which at the same time the author will also get the transmittance value. Next, using this absorbance value, the author will obtain the absorption coefficient data and also extinction coefficient data, k . after that, by using Kramers - Kronig method, value of refraction index will be obtain. All these data will then be inserted into the coding for the ATHENA. For every thickness, these software will then evaluate the performance the DSSC for every thickness.

3.4 Gantt Chart

To ensure the consistency of this project, a gantt chart has been produce to ensure that at the specific time, the target had been achieved. This gantt chart will also function as a rough guidance to the author. The gantt chart is available in the APPENDIX section. This gantt chart is for the first term. For the second term, the author used project flowchart.

3.5 Equipment

For now, these are the expected equipment needed for this experiment:

1. Dye Sensitized Solar Cell

3.6 Atlas software

ATLAS is a simulator that able to simulate the electrical, optical and thermal behavior of the semiconductor devices based on virtual fabrication of its physical structure. It is able to provide the I-V characteristic, photogeneration mapping and spectral response. For silicon based technologies, S-Pisces is used together with the ATLAS as a device simulator that incorporates both drift-diffusion and energy balance transport equations [17]. In addition, Luminous is also used with the ATLAS as an advanced device model that able to model light absorption and photogeneration in planar and non-planar semiconductor devices.

3.7 Project Flowchart

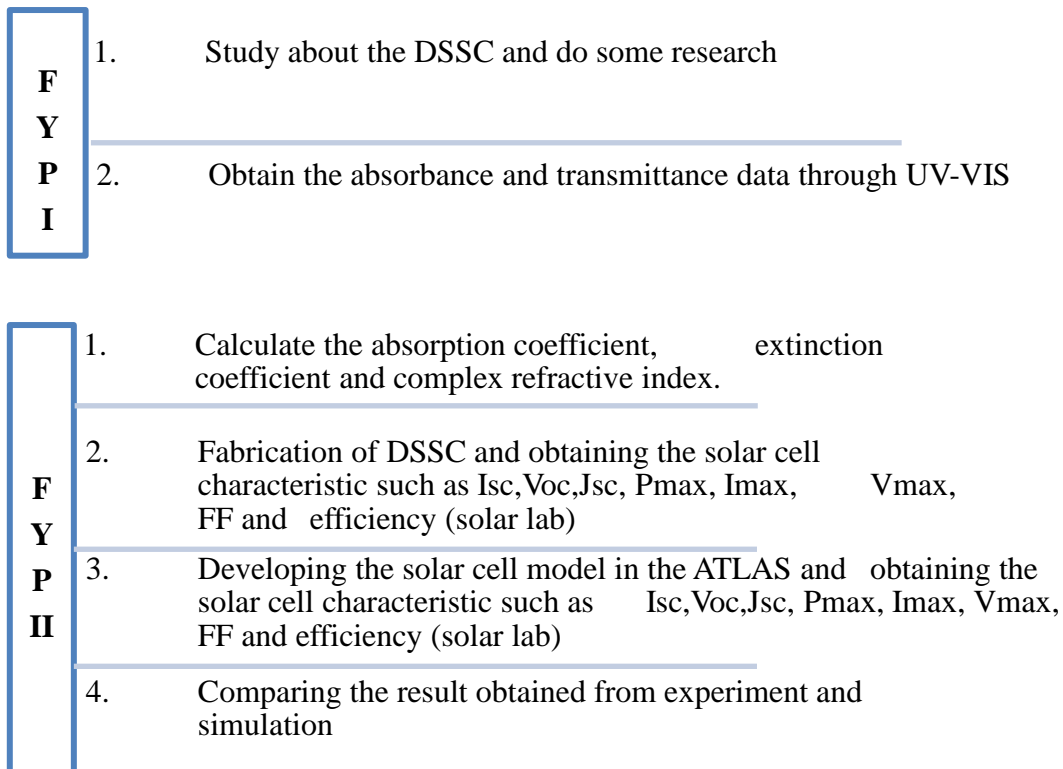


Figure 4: Project flowchart

3.8 Obtaining Complex Refractive Index using UV-Vis Absorption Spectroscopy

Steps for obtaining refractive index:

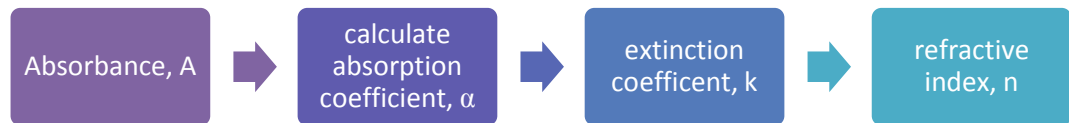


Figure 5: Flow for obtaining the refractive index

Absorbance and transmittance are obtained using UV-VIS method. Firstly, the sample and the reference have been put in the chamber. Next, wavelength range of the light has been set from 300nm until 800nm. Then, the chamber is closed and measurement is started. The author calculates absorbance value for every wavelength which ranges from 200nm until 800nm. Absorption coefficient can be obtained using absorbance data. Next, these sets of absorption coefficient values are used to calculate the extinction coefficient. These two values are then used to calculate the refractive index, n .

3.9 Fabrication of DSSC

For this part, the author has the collaboration with the postgraduate student to accomplish this experiment. This experiment has two parts:

1. Preparation

Preparing the things need to be use in the experiment such as TCO glass, TiO_2 paste, and dye.

2. Screen printing

Through this method, the TiO_2 paste had been printed on the TCO surface. The author made three different thicknesses which are 6 μm , 12 μm and 18 μm . One pass will make a 6 μm of thickness. So eventually, we need to make 2 passes for 12 μm and three passes for 18 μm . This TiO_2 paste consists of nanoparticles only.

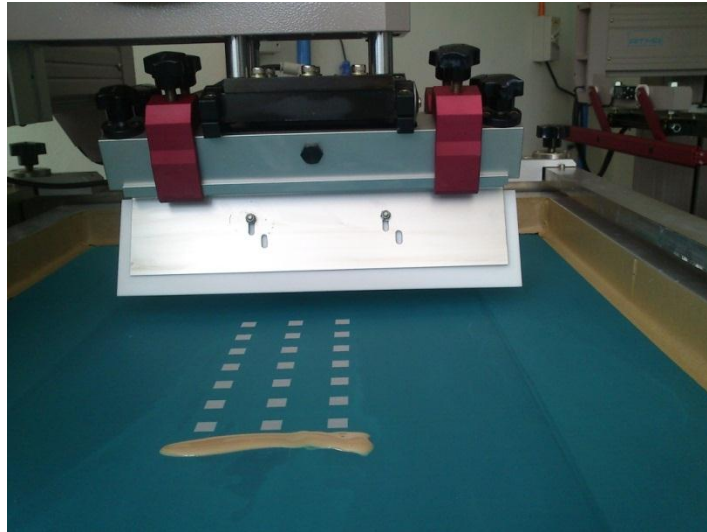


Figure 6: screen printing process

3. Dry the printed TCO glass

For this process, the TCO glass will be dried out before proceed to the next step. This printed TCO will be dry using belt furnace with the temperature inside the furnace is around 550 °C.



Figure7: Belt furnace

4. Dye soaking

TCO glass will be arranged in a special box. After that, dye solution will be poured into the box until full. Next, the box will be closed for 15 hours. This is to ensure that the soaking process is fully complete. However, this soaking process is varies with the type of dye used. This soaking process may takes longer up to 48hours.

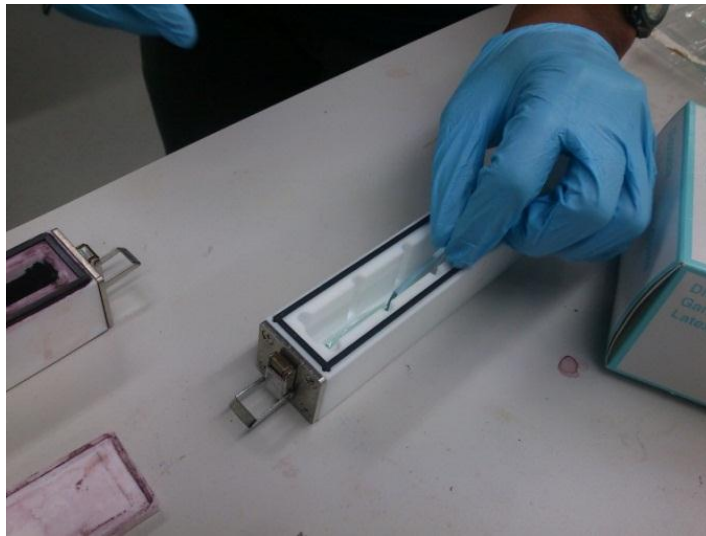


Figure 8: arranging the dye into the box



Figure 13: filling in the dye solution

5. Sandwiching the electrodes

After 15 hours has been passed, the glass will be taken out from the box. Next, it will go through the next process which is sandwiching the dye by another TCO glass that has a small hole in the center. These two glasses will be paste together using a plastic gasket that has been placed in between these

two glasses. Next, through the heat press process, these two glasses will be stick together. After that, a cold press is used to cool down the heated glass. Next is the electrolyte filling process which will be injected through the small hole using the pump and vacuum dessicator. Last part for this step is to seal the small hole by using the aluminum foil.



Figure 10: hot press process



Figure 11: cold press process



Figure 12: electrolyte filling process



Figure13: hole sealing process

3.10 Simulation of solar cell

The Dye-Sensitized Solar Cell consists of two regions which are the bulk heterojunction region and the electrolyte region. The bulk heterojunction region is TiO_2 particles interconnected with dye which is light absorbing material with three different thicknesses of film which are $6\mu\text{m}$, $12\mu\text{m}$ and $18\mu\text{m}$. Electrolyte region consists of redox solution with the thickness of $25\mu\text{m}$.

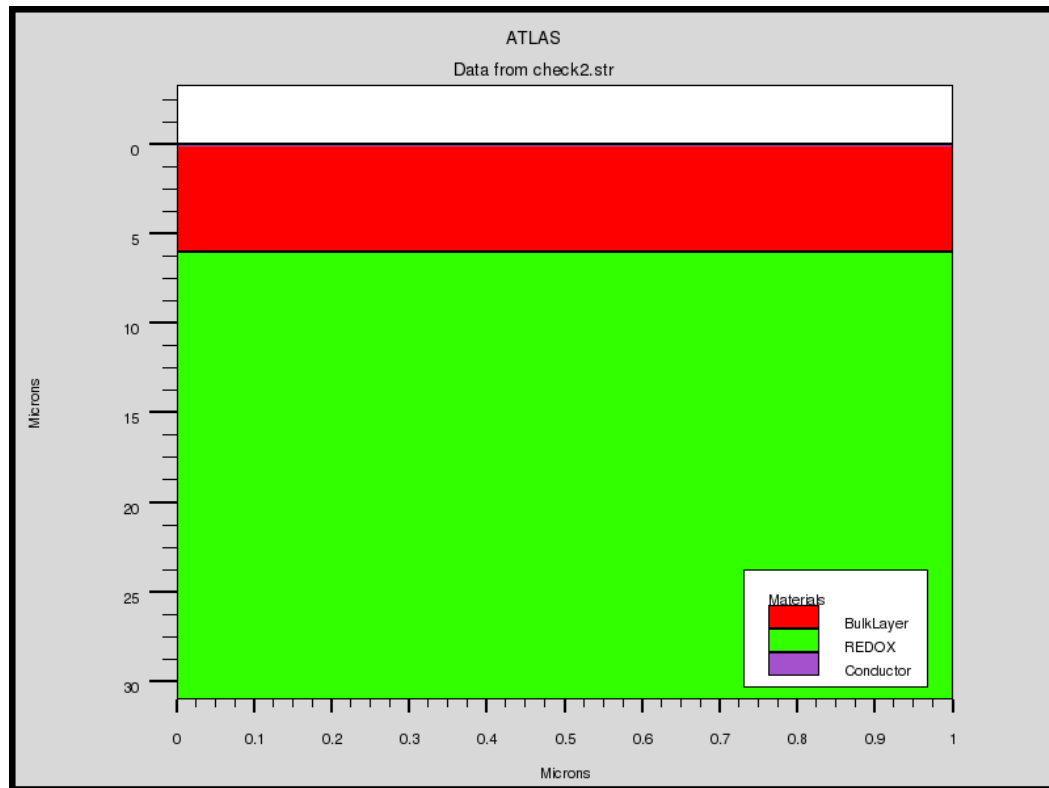


Figure 14: DSSC structure for $6\mu\text{m}$ in ATLAS

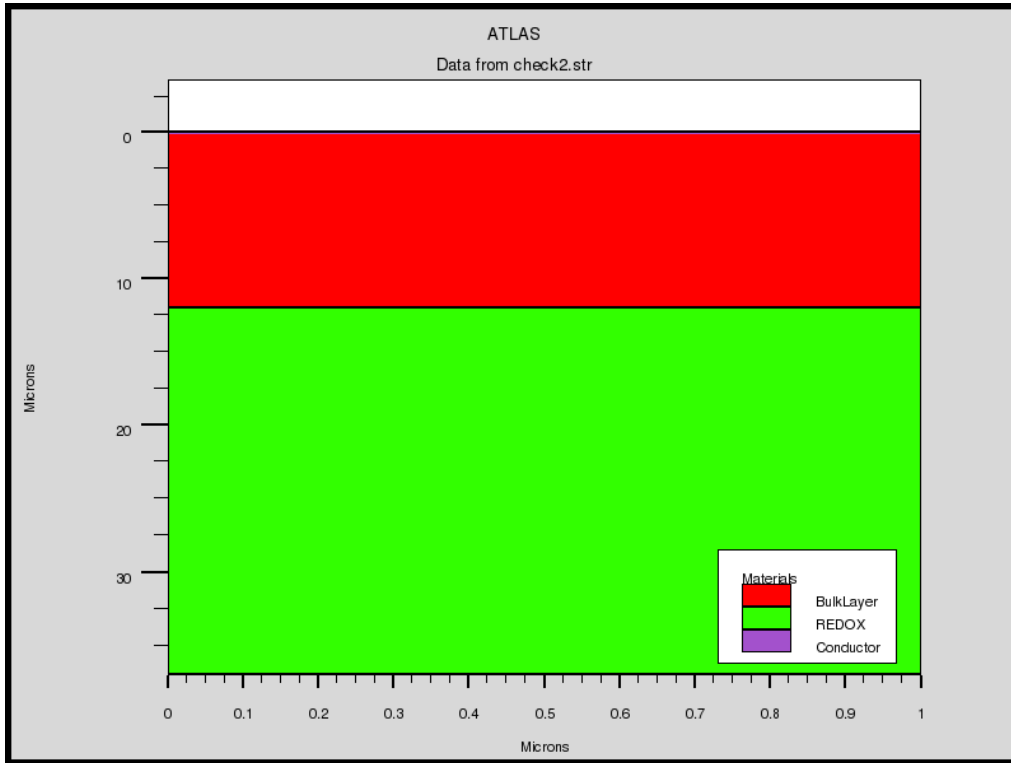


Figure 15: DSSC structure for 12 μ m in ATLAS

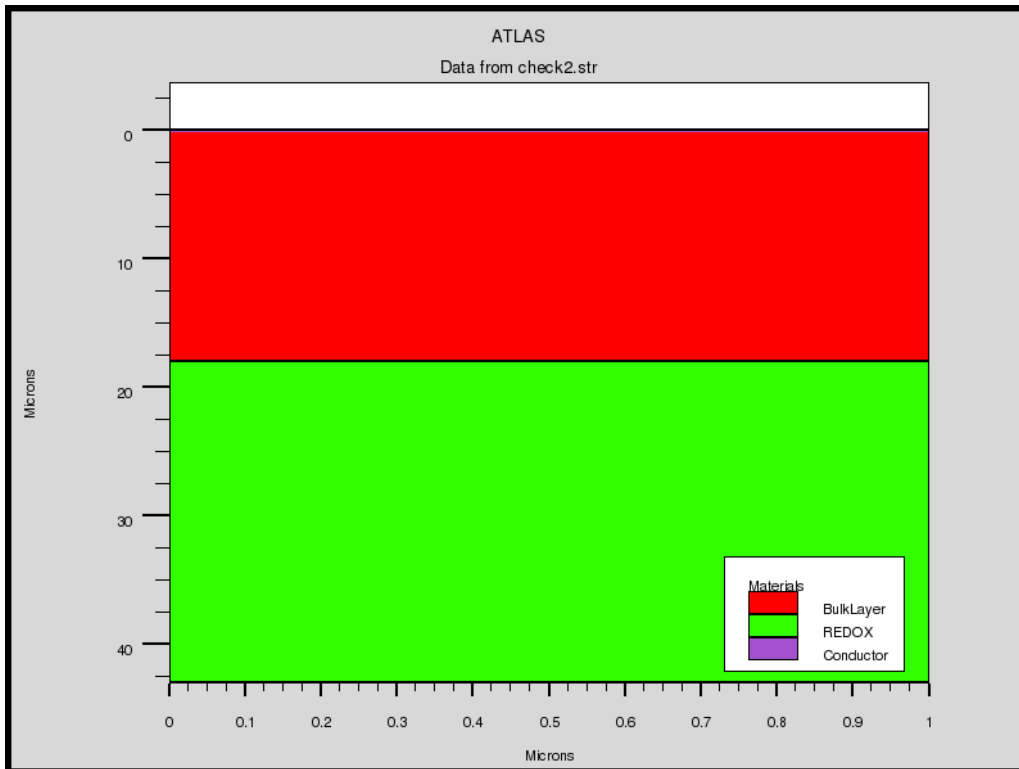


Figure 16: DSSC structure for 18 μ m in ATLAS

We set the anode and cathode to be an electrical contact in order to simulate the electrical properties with the work function is set to be 4.4eV. After that, the author used Langevin recombination model to describe the recombination process. Material used in the DSSC was not listed in the ATLAS. Thus, the material parameters are set according to table below:

Material	Material parameter	Value
Bulk layer	Material class	Semiconductor
	permittivity	50
	Affinity	4 eV
	Energy Gap	1.5eV
	Conduction band density	$2.8 \times 10^{19} \text{ cm}^{-3}$
	Valence band density	$1.9 \times 10^{19} \text{ cm}^{-3}$
	Electron mobility	$0.3 \text{ cm}^2/\text{V.s}$
	Hole mobility	$3 \times 10^{-4} \text{ cm}^2/\text{V.s}$
REDOX	Material class	Semiconductor
	permittivity	3.5
	Affinity	3.4 eV
	Energy Gap	0.93 eV
	Conduction band density	$2.8 \times 10^{19} \text{ cm}^{-3}$
	Valence band density	$1.9 \times 10^{19} \text{ cm}^{-3}$
	Electron mobility	$7.07 \times 10^{-2} \text{ cm}^2/\text{V.s}$
	Hole mobility	$7.07 \times 10^{-2} \text{ cm}^2/\text{V.s}$

Table 1: Material Parameter defined in ATLAS

3.11 Obtaining IV Characteristics of the Dye-Sensitized Solar Cell

ATLAS is also used to simulate the IV characteristic of the device. Before that, some set up need to be done. Source beam is located in the middle of the solar cell and $2\mu\text{m}$ from the cell. Angle of the beam is 90° which is normal to the cell. Air Mass 1.5 (AM 1.5) is used to test the solar cell which is the standard spectrum at the earth surface. Parameters are listed in the table 2.

Parameter	Value
Location of the beam source (x,y)	(0.5,-2.0)
Angle of beam	90.0°
Solar spectrum	AM 1.5

Table 2: Beam parameter set up in ATLAS

Chapter 4

RESULT AND DISCUSSIONS

4.1 Determination of complex refractive index

TiO₂ thickness is varies with three different thicknesses which are 6 μ m, 12 μ m and 18 μ m. the temperature is fixed at 700°C. The absorbance data which is obtained from the UV-Vis method showed the figure 17.

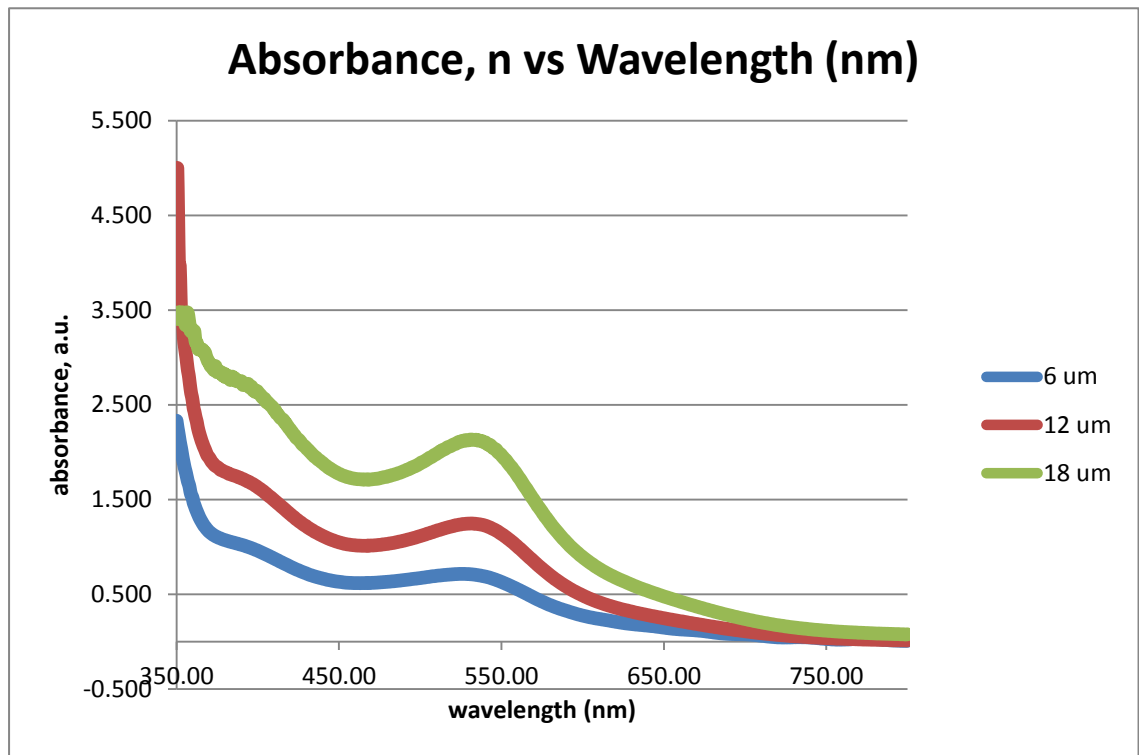


Figure 17: Absorbance of TiO₂ layer as the function of wavelength

From the absorbance data that the author gets, absorption coefficients are then calculated by using the equation 6. The result of the absorption coefficient is then plotted as below:

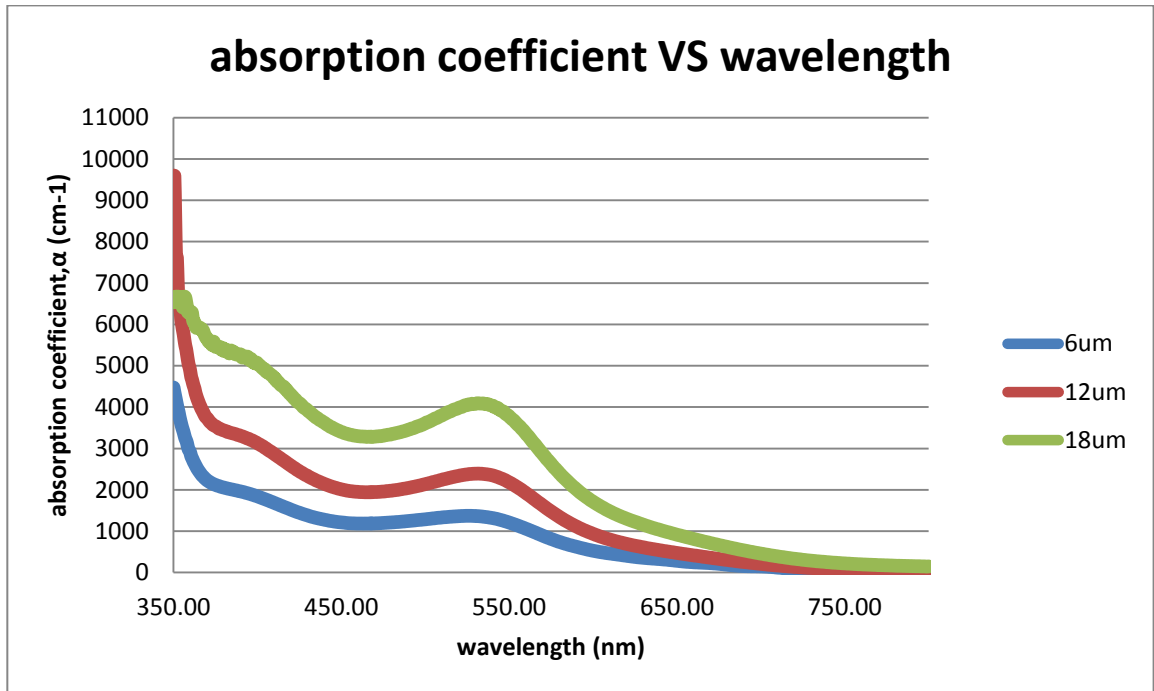


Figure 18: Absorption coefficient of TiO₂ layer as the function of wavelength

By using these absorption data above, the author then calculate the extinction coefficient using equation 8. Lastly, refractive index is determined using the kramers-kronig equation calculated using MATLAB.

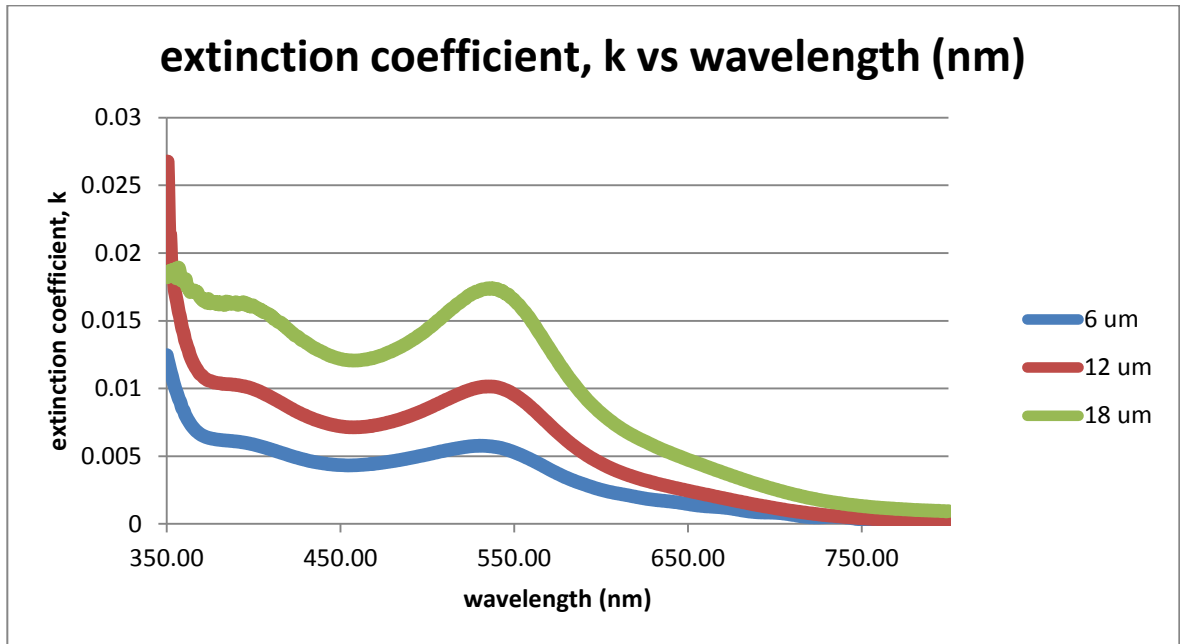


Figure 19: Extinction coefficient of TiO₂ layer as the function of wavelength

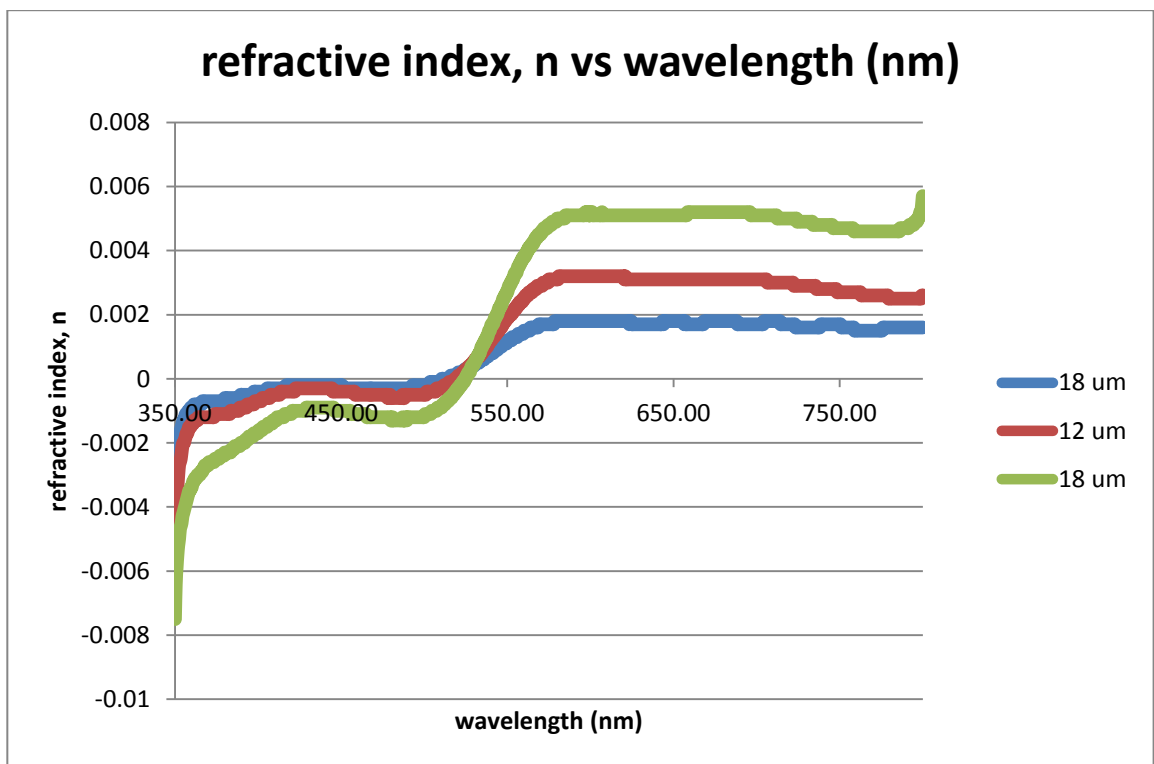


Figure 20: Refractive index of TiO₂ layer as the function of wavelength

4.2 Dye-Sensitized Solar Cell parameter variation for simulation and experimental

The Dye-Sensitized Solar Cell was used to simulate the effect of TiO₂ layer by varying the thickness of the TiO₂ layer. Simulation results shows that TiO₂ layer with the thickness of 18 μ m has the best efficiency with the value 4.27%.

SIMULATION							
Thickness (um)	Isc(mA)	Voc(V)	Pmax(mW)	Vpmax(V)	FF	efficiency	Imp(mA)
6	8.95	0.73	2.23	0.30	0.34	2.23	7.44
12	11.61	0.74	3.06	0.30	0.36	3.06	10.21
18	15.55	0.75	4.27	0.35	0.37	4.27	12.20

Table 3: Summary of DSSC performance for three thicknesses (simulation)

Experiment also show that TiO₂ layer with the thickness of 18 μ m has the best efficiency with the value 3.10%.

EXPERIMENT							
Thickness (um)	Isc(mA)	Voc(V)	Pmax(mW)	Vpmax(V)	FF	efficiency	Imp
6	7.45	0.64	2.31	0.40	0.49	2.31	5.85
12	9.26	0.58	2.77	0.38	0.51	2.77	7.34
18	10.30	0.66	3.10	0.39	0.46	3.10	8.036

Table 4: Summary of DSSC performance for three thicknesses (experiment)

The maximum short circuit current, Isc and open circuit voltage, Voc affected the Fill Factor as shown in figure 25. For experiment, Fill Factor is the lowest for the thickness of 18 μ m which differ from simulation which says that 12 μ m thickness has the lowest Fill

Factor. This difference happened because Fill Factor is the ratio between the maximum power to the product of open circuit voltage and short circuit current. Short circuit current, I_{sc} variation for the experiment is not much compared to the simulation. Thus, it gives the different result for the lowest Fill Factor.

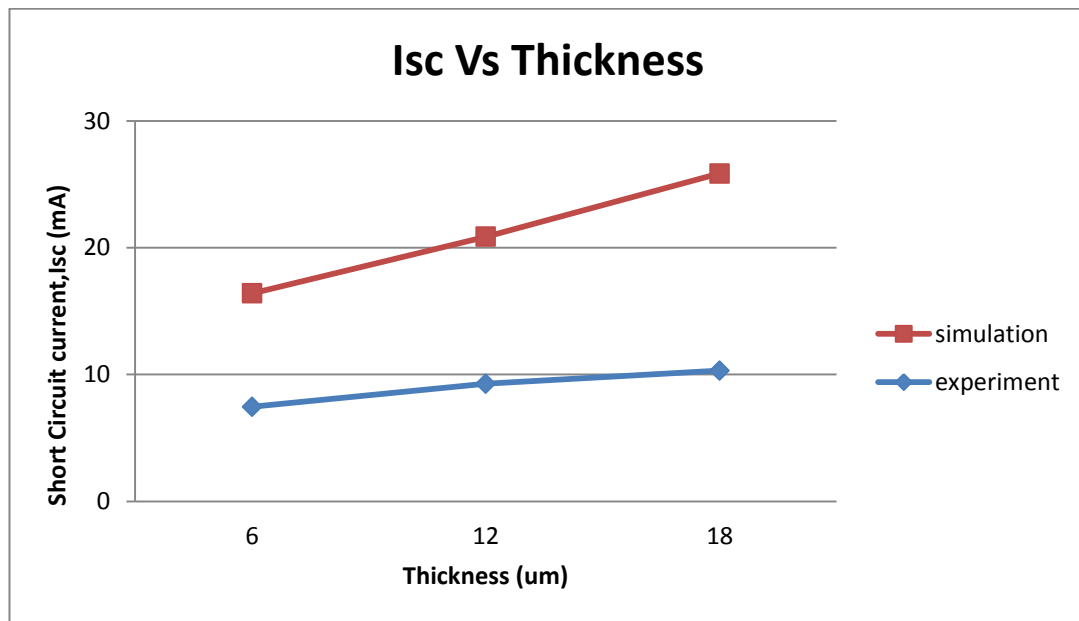


Figure 21: Effect of TiO_2 thickness on the short circuit current, I_{sc} of the DSSC

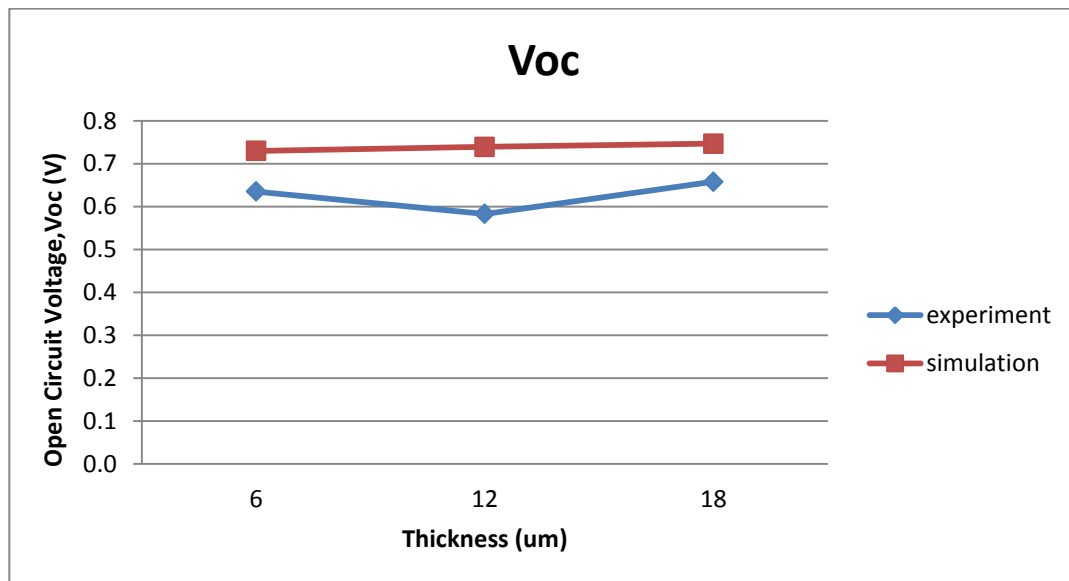


Figure 22: Effect of TiO_2 thickness on the open circuit voltage, V_{oc} of the DSSC

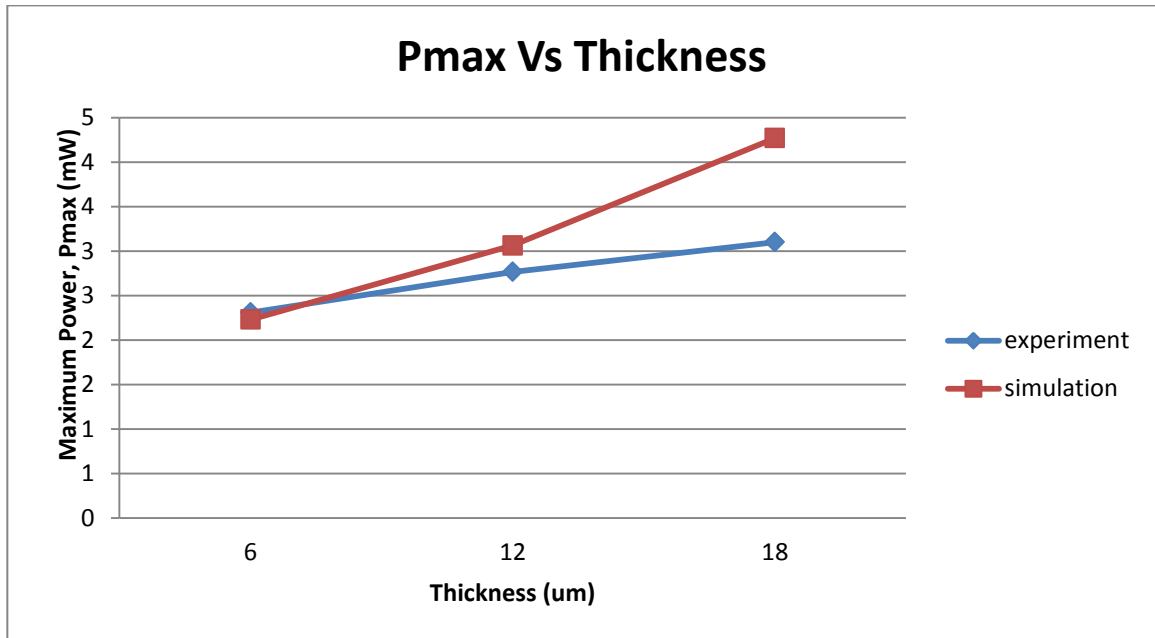


Figure 23: Effect of TiO₂ thickness on the maximum power, Pmax of the DSSC

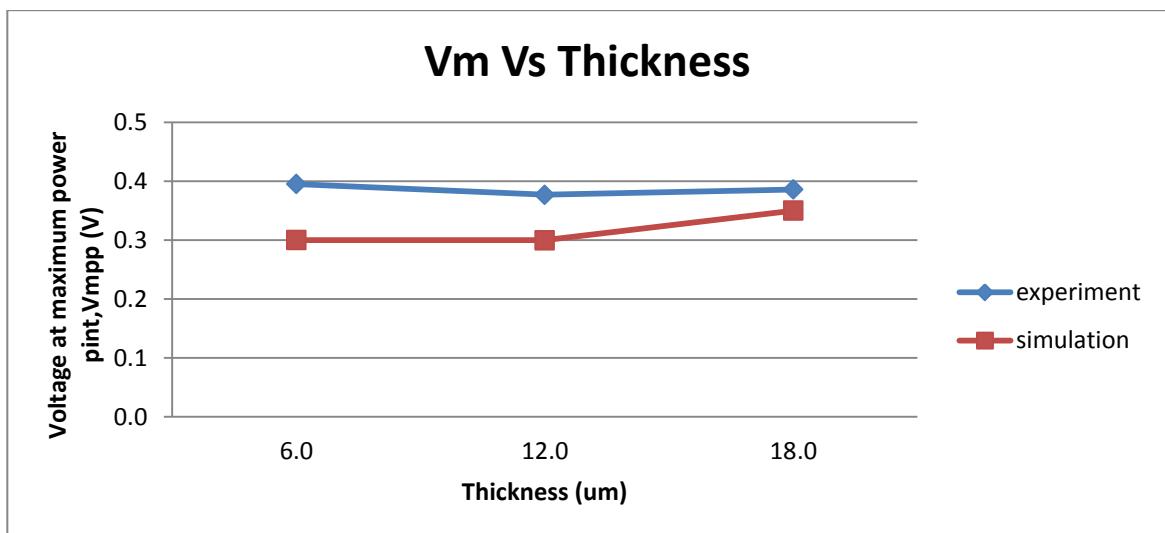


Figure 24: Effect of TiO₂ thickness on the maximum voltage, Vm the DSSC

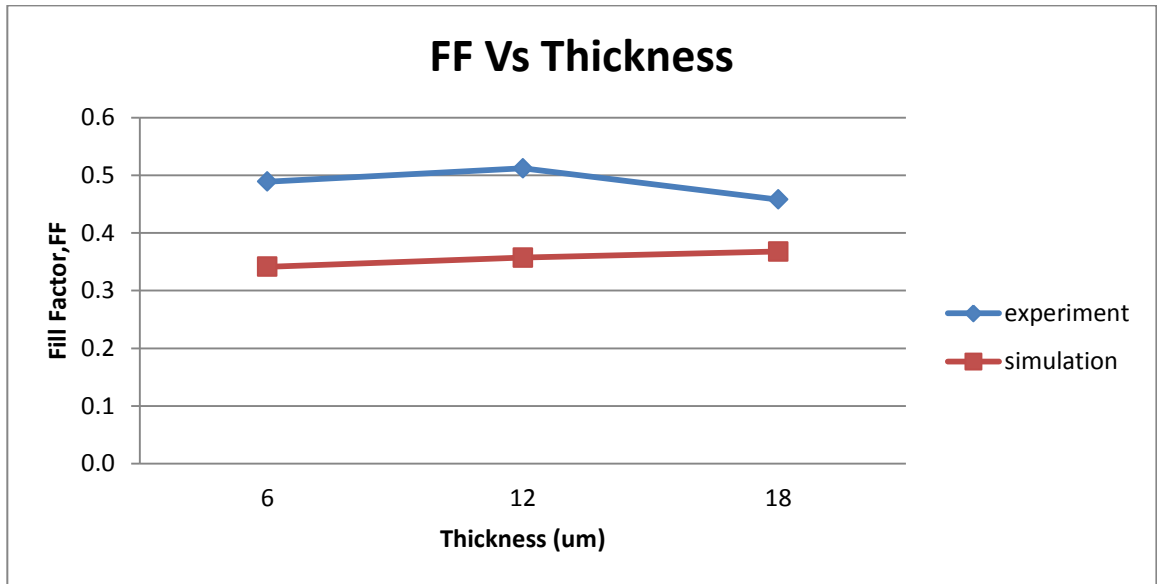


Figure 25: Effect of TiO₂ thickness on the Fill Factor, FF of the DSSC

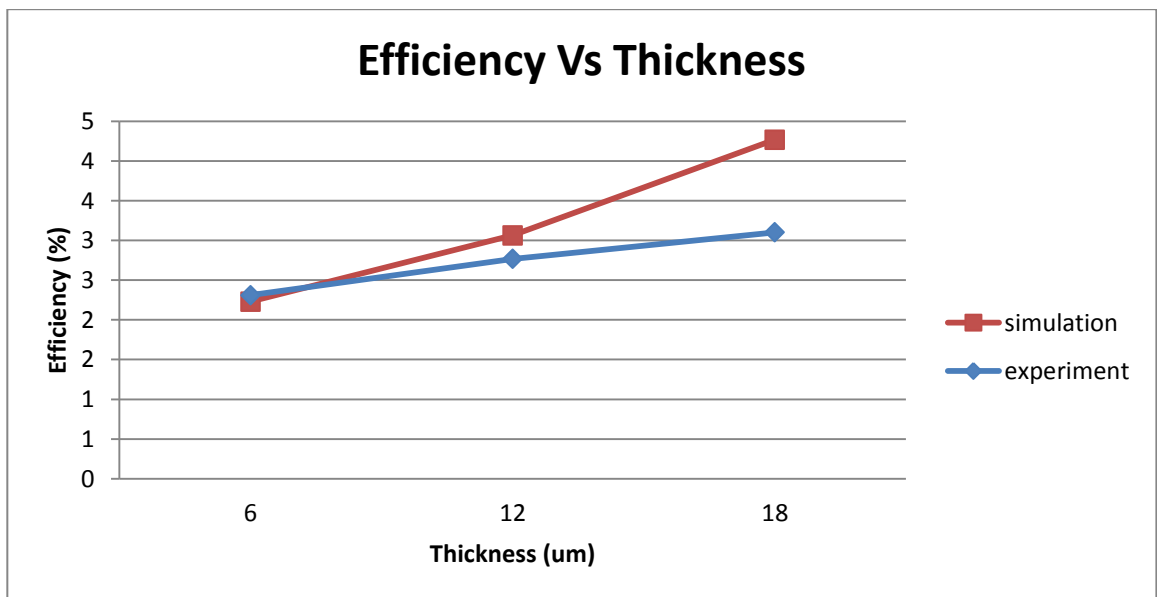


Figure 26: Effect of TiO₂ thickness on the efficiency of the DSSC

4.2.1 IV characteristics of the Dye-Sensitized Solar Cell

4.2.1.1 IV characteristics for simulation

By plotting the current and voltage, there are significant differences for every thickness with 18 μm has the highest curve compared to the other two thicknesses.

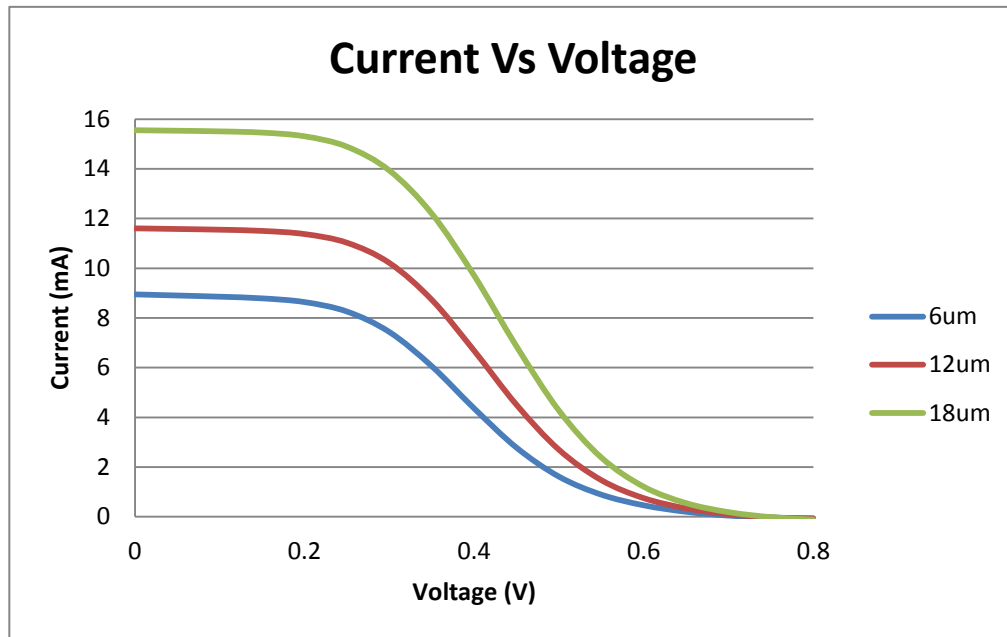


Figure 27: Comparison of Current Vs Voltage for three thicknesses

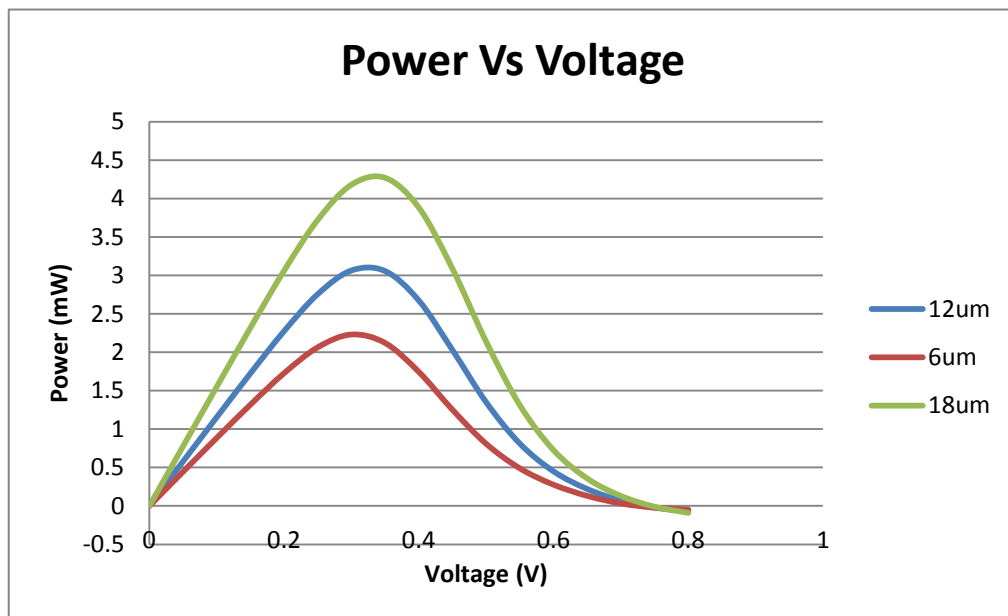


Figure 28: Comparison of Power Vs Voltage for three thicknesses

4.2.1.2 IV characteristics for experiment

Experimental result is same as the simulation result with the 18 μm give the highest curve. However, the values difference between three thicknesses is quite close compared to the simulation result.

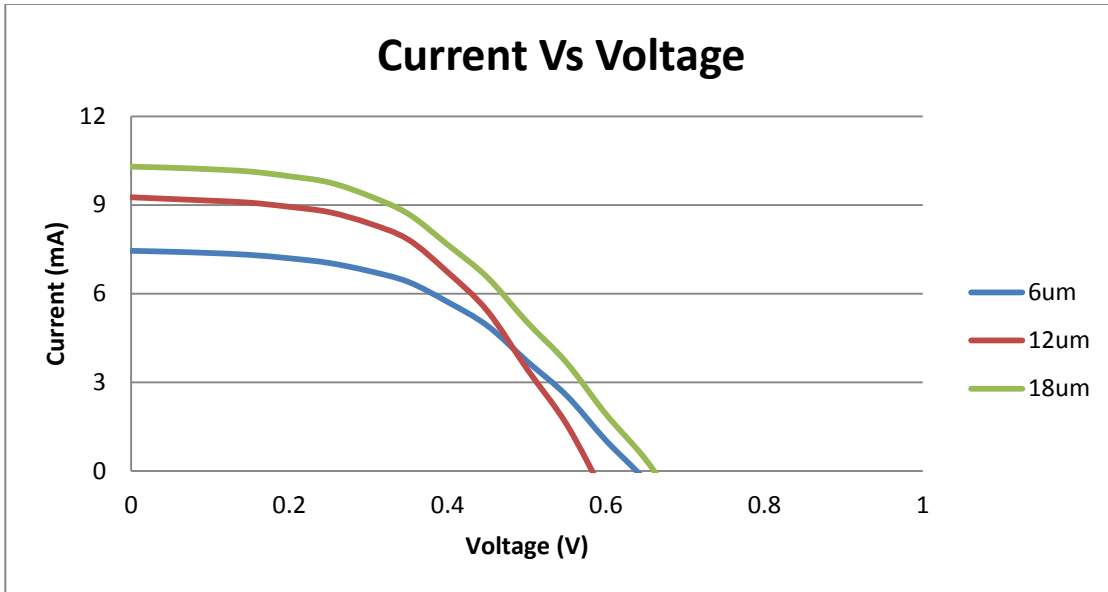


Figure 29: Comparison of Current Vs Voltage for three thicknesses

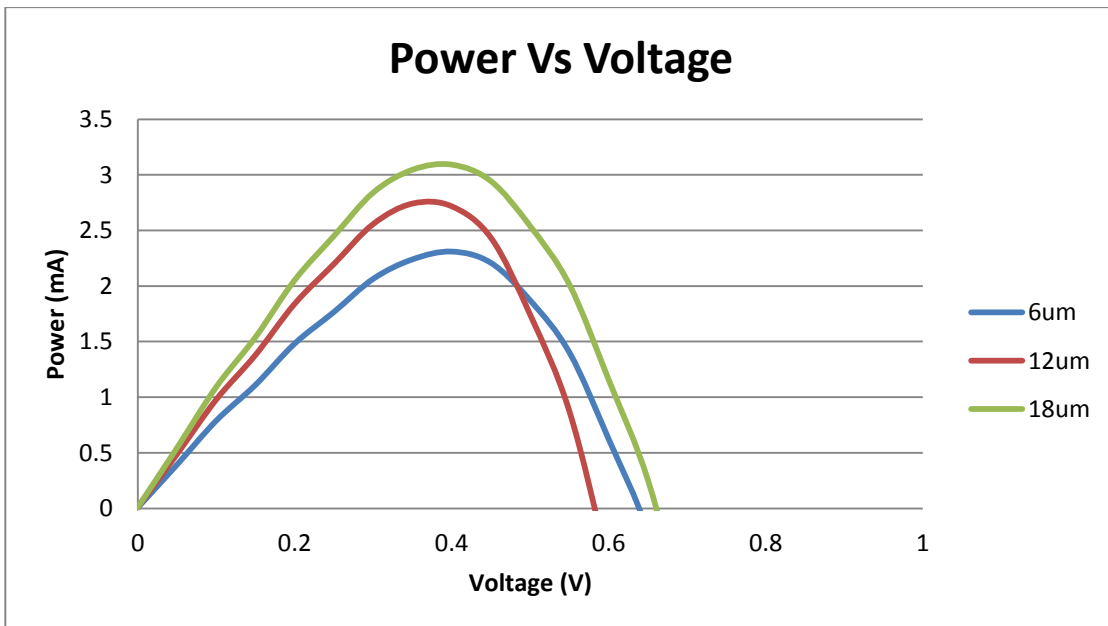


Figure 30: Comparison of Current Vs Voltage for three thicknesses

Chapter 5

Conclusion and recommendation

This paper generally undergoes research on DSSC efficiency by making TCO variation thickness as the variable. By increasing the thickness, more electrons can flow through but the resistivity in the TCO itself cannot be ignored.

Firstly, the student had performed the calculation of the refractive index used in Dye-Sensitized Solar Cell. Calculated refractive index has shown the effect of varying the thickness of TiO_2 layer. Thicker layer of TiO_2 resulted to higher value of refractive index.

This has been done at solar lab and the data obtained will be visualized in the form of graph. In order to obtain accurate data, these experiments need to be conducted in a very careful way since DSSC is very small. A deep understanding on DSSC mechanism is a must since it will affect the experimental result later on.

From the experimental result, 18 μm has the best efficiency compare to 6 μm and 12 μm . Simulation result also gives the same result which is 18 μm gives the best efficiency compared to 6 μm and 12 μm . The author first assumption is that thicker layer of TiO_2 will give the opportunity for the dye to absorb more sunlight and thus increase the dye-sensitized solar cell (DSSC) efficiency. Simulation and experimental result prove this.

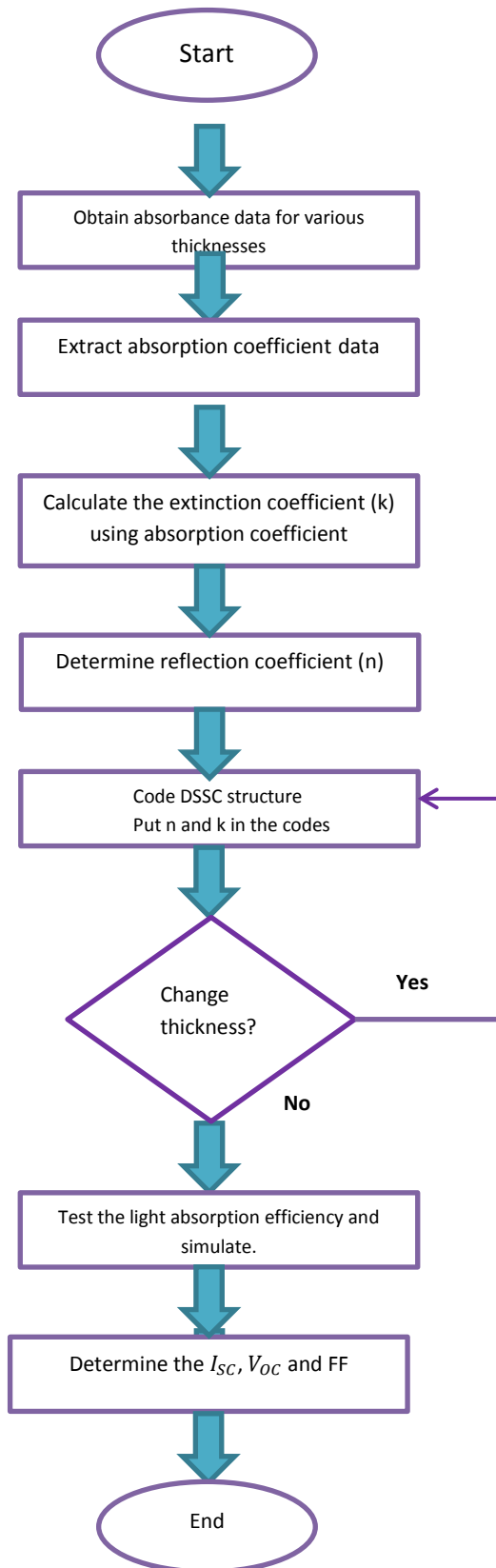
However, even though both simulation and experimental result point out the same thickness for the best efficiency, the efficiency value between simulation and experimental is quite big. Simulation shows that thickness of 18 μm gives efficiency of 4.27% while the experimental gives 3.10%. It gives 37.6% different between these two results. This large difference may happen due

to error made during fabrication of Dye-Sensitized Solar Cell in the lab and also some assumptions made during simulation process. In order to get more accurate result, repetitive experiment with at least three samples for every thickness is suggested.

Lastly, both experimental and simulation are able to show the pattern of the effects of the thickness variations in TiO_2 layer.

APPENDICES

APPENDIX A: EXPERIMENT FLOWCHART



APPENDIX B: Gantt chart

No	Detail	1	2	3	4	5	6	Mid semester break	7	8	9	10	11	12	13	14	
1	Selection of Project Title:	█															
2	Preliminary Research Work: Research related to topic		█	█	█												
3	Submission of Extended Proposal					█	█										
4	Project work:																
	i) Familiarization with related instrument									█	█						
	ii) Operating procedure of the project									█	█						
5	Proposal Defense									█	█	█					
6	Project Work continues:																
	i) Test the software												█	█	█		
	ii) Obtaining data												█	█	█		
7	Submission of draft for interim report															█	
8	Submission of interim Report Final Draft																█

APPENDIX C: MATLAB CODE [16]

```

function imchi=kkimbook(omega,rechi,alpha)
%The program inputs are 1) omega, vector of the frequency
%(or energy) components, 2) imchi, vector of the imaginary
%part of the susceptibility under examination, and 3) alpha,
%the value of the moment considered. The two vectors
%1) and 2) must have the same length.
%The output is the estimate of the real part as obtained
%with K-K relations.
%In order to use this program, save the whole text contained
%in this section in a file and name it kkrebook.m

load omega.csv
omega=f;
%omega(:,1)=[]; %eliminate first column to get omega vector
if size(omega,1)>size(omega,2);
omega=omega';
end;

load kenam.csv
imchi=kenam;
%imchi(:,1)=[];
if size(imchi,1)>size(imchi,2);
imchi=imchi';
end;

%Here the program rearranges the two vectors so that,
%whichever their initial shape, they become row vectors.
g=size(omega,2);
%Size of the vectors.%
rechi=zeros(size(imchi));
%The output is initialized.
a=zeros(size(imchi));
b=zeros(size(imchi));
%Two vectors for intermediate calculations are initialized
deltaomega=omega(2)-omega(1);
%Here we compute the frequency (or energy) interval

alpha=0;
j=1;
omega=j*omega;
beta1=0;
for k=2:g;
b(1)=beta1+imchi(k)*omega(k)^(2*alpha+1)/....
(omega(k)^2-omega(1)^2);
beta1=b(1);
end;
rechi(1)=2/pi*deltaomega*b(1)*omega(1)^(-2*alpha);
%First element of the output: the principal part integration
%is computed by excluding the first element of the input

```

```

j=g;
alpha1=0;
for k=1:g-1;
a(g)=alpha1+imchi(k)*omega(k)^(2*alpha+1)/...
(omega(k)^2-omega(g)^2);
alpha1=a(g);
end;
rechi(g)=2/pi*deltaomega*a(g)*omega(g)^(-2*alpha);
%Last element of the output: the principal part integration
%is computed by excluding the last element of the input
for j=2:g-1;
%Loop on the inner components of the output vector.
alpha1=0;
beta1=0;
for k=1:j-1;
a(j)=alpha1+imchi(k)*omega(k)^(2*alpha+1)/...
(omega(k)^2-omega(j)^2);
alpha1=a(j);
end;
for k=j+1:g;
b(j)=beta1+imchi(k)*omega(k)^(2*alpha+1)/...
(omega(k)^2-omega(j)^2);
beta1=b(j);
end;
rechi(j)=2/pi*deltaomega*(a(j)+b(j))*omega(j)^(-2*alpha);
end;
%Last element of the output: the principal part integration
%is computed by excluding the last element of the input

```


APPENDIX D: ATLAS CODING

```
go atlas simflags="-P 1"
mesh width=1e12
x.mesh l=0.00 s=0.5
x.mesh l=1.00 s=0.5
y.mesh l=0.00 s=0.05
y.mesh l=12.00 s=0.05
y.mesh l=37.00 s=0.05
region number=1 user.material=BulkLayer y.min=0.00 y.max=12.00
region number=2 user.material=REDOX y.min=12.00 y.max=37.00
electrode name=anode top
electrode name=cathode bottom
contact num=1 workf=4.4
contact num=2 workf=4.4
model langevin singlet s.dissoc
model print
material material=BulkLayer user.default=Organic
user.group=Semiconductor
material material=REDOX user.default=Organic
user.group=Semiconductor
material material=BulkLayer permi=50 affinity=4.0 eg300=1.5 \
nc300=2.8e19 nv300=1e19
material material=REDOX permi=3.5 affinity=3.4 eg300=1.8 \
nc300=2.8e19 nv300=1e19
material material=BulkLayer index.file=dye400.nk
material material=REDOX index.file=iodide.nk
material material=REDOX qe.exciton=1.0
material material=REDOX knrs.exciton=1.82694e6 lds.exciton=0.0 \
taus.exciton=1.0e20 rst.exciton=1.0
material material=REDOX a.singlet=2 s.binding=0.004
mobility material=BulkLayer mun=0.3 mup=450e-4
mobility material=REDOX mun=1350 mup=450
save outf=check1.str
beam num=1 x.origin=0.5 y.origin=-2.0 angle=90.0 AM1.5
output band.par con.band val.band e.mob h.mob opt.int
probe name=inten beam=1 intensity
method climit=1e-4 maxtrap=0
#IV Characteristics
solve init
solve previous
log outfile=dark_current.log
solve vcathode=-1 vstep=0.05 vfinal=1 name=cathode
log off
solve init
solve prev
solve b1=1
log outf=light_current.log
solve vcathode=-1 vstep=0.05 vfinal=1 name=cathode b1=1
```

```

log off
save outf=check2.str
extract init infile="light_current.log"
extract name="Isc" y.val from curve(v."cathode", (i."cathode"))
where x.val=0
extract name="Voc" x.val from curve(v."cathode", (i."cathode"))
where y.val=0
extract name="Jsc (mA/cm2)" abs($"Isc")*1e-1
extract name="Power" curve(v."cathode", (v."cathode" *
i."cathode"
*(-1))) \
outf="P.dat"
extract name="Pmax" max(curve(v."cathode",
(v."cathode"*i."cathode"*(-1))))
extract name="V_Pmax" x.val from
curve(v."cathode", (v."cathode"*i."cathode")) \
where y.val=(-1)*$"Pmax"
extract name="Fill Factor" ($"Pmax"/(abs($"Isc")*$"Voc"))
extract name="intens" max(probe."inten")
extract name="Eff" (($Pmax/($"intens"*1e4))*100)
tonyplot dark_current.log -overlay light_current.log
tonyplot P.dat
tonyplot check2.str
quit

```

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