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Simulation of Electron Diffusion Coefficient Interpretation on the Optimum Thickness of TiO_2 Photoanode in Dye-Sensitized Solar Cell (DSSC)

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Abstract. DSSC is a natural dye-based organic solar cell composed of layers of semiconductor (photoanode), dye, electrolyte, and the counter electrode. The photoanode layer on DSSC acts as a dye binder and can pass on excited electrons to the electrode counter. This component is one of the keys to improve the DSSC performance. The TiO_2 material has been used widely as a photoanode due to its high stability to light so that at its optimum thickness it can pass well the sunlight energy on the surface of the DSSC. When the sunlight energy impinges to DSSC for relatively long time, it can increase the working temperature. Theoretically, the increase in the working temperature of the DSSC causes an increase in the electron diffusion coefficient in the DSSC, thus affecting its performance. Therefore, the interpretation of an increase in the electron diffusion coefficient due to an increase in the thickness and working temperature in DSSC is essential to be studied. In this article, a simulation of the determination of the optimum thickness of TiO_2 photoanode was carried out. We studied the effect of electron diffusion coefficient on the DSSC open voltage at the optimum thickness. The highest electron diffusion coefficient in this simulation was 9.65×10^{-3} cm^2/s with current density of 0.0145 A/cm^2, voltage of 0.3411 V, power of 0.0020 $V \cdot A/cm^2$, and efficiency of 2.000%. We found that the higher the electron diffusion coefficient, the open voltage of DSSC increased so that its performance also increased.

Keywords: Thickness of TiO_2 photoanode, working temperature, electron diffusion coefficient, DSSC performance

1. Introduction

Increasing population in the world causes greater world energy demand [1]. So far, the world energy needs have been supplied by conventional energy sourced from coal, petroleum, and natural gas. This conventional energy has brought great progress in the economic field but its excessive use can damage the environment and human health [2]. This condition triggers the idea to utilize the potential of alternative energy as a substitute for conventional energy because the use of alternative energy can be one solution to overcome the problem of environmental damage [3]. Some alternative energy sources that can be utilized include biomass, wind, solar light, hydropower, and geothermal [2,4]. From some of these alternative energy sources, sunlight energy is one of the choices and solutions to depleting fossil energy sources because the amount of energy supplied by the sun to the earth is very abundant, reaching nearly four million annually [5]. This solar light energy is basically can be converted into electrical energy using a device that is a solar panel. Based on its function, solar panel devices are often referred to as photovoltaic cells (PV cells). Initially, the developed PV cells were made from monocrystalline or polycrystalline silicon (Si) [6].

Si is one of the first intrinsic semiconductor materials applied in the manufacture of PV cells with the advantage of having high-efficiency so that the first generation of silicon cell technology is based on silicon. Furthermore, second generation solar cell technology with a thin film based on organic semiconductors was developed, and the third generation developed natural dye-based dye solar cells known as dye-sensitized solar cells (DSSC) [7].

DSSC utilizes semiconductor materials used as dye binders. One of the semiconductor materials that widely be used is titanium dioxide (TiO_2) [8,9]. TiO_2 is a semiconductor material that has unique properties including high stability against light [10] and wide energy bandgap (3.2 eV) [11]. TiO_2 shows a high stability under light and can be used to pass on the excited electrons toward the counter electrode.

The study of micrometer scale of DSSC modeling electrode with various thicknesses has been conducted to find the maximum power generated by the solar window [11]. In 2011, the calculation of DSSC parameters had been reported [12]. Furthermore, in 2016 an experimental study was carried out on the effect of the thickness of the micrometer on TiO_2 transparent working electrodes as a DSSC application [7]. An experiment of various thicknesses was reported previously on TiO_2 as a photoanode of DSSC [13] while a mathematical modeling had been carried out to describe an array of PV cells connected with a variable resistor [14]. Furthermore, an effect of extreme temperatures on the performance of DSSC was also reported [15].

Based on these studies, the thickness of TiO_2 photoanodes and the effect of working temperature are the key to improving DSSC performance. The longer time of DSSC to be exposed under sunlight, the working temperature will increase. Theoretically, the increase in working temperature affects the increasing in diffusion coefficient of the electron [16]. This subsequently affects the performance of DSSC. Therefore, in addition to the thickness optimization of TiO_2 photoanode, the effect of increasing the electron diffusion coefficient on DSSC due to the increase in work temperature needs to be studied.

2. Methods

In this study, the simulation was carried out to obtain the optimum thickness of TiO_2 photoanode. This optimum thickness could be analyzed based on the results of the electrical current to the electrical voltage (J-V) and the electrical power to the electrical voltage (P-V) curves. The simulated thickness was in the range of 1 nm to 20 µm. The simulation activities were conducted using the appropriate input parameters in Table 1.

Table 1. Input parameters

Parameter	Value	Remarks	Reference
k	$1.381\text{x}10^{-23}$ J/K	Boltzmann constant	
q	$1.602\ \text{x}10^{-19}$ C	electron charge	
L	$2.2361\ \text{x}10^{-3}$ cm	length of electron diffusion	[12]
∝	5000 cm^{-1}	absorption coefficient	[9, 12]
m	4.5	ideal factor	[9,11,12]
D	$2.3\text{x}10^{-5}\ cm^2/s$	diffusion coefficient	[9]
n_0	10^{16} elekton/cm^2	electron concentration	[9,11,12]
τ	0.01 s	lifetime	[9, 11,12]
Φ	$1\text{x}10^{17}\ cm^{-2}s^{-1}$	sunlight intensity	[9, 11]
μ	0.3 cm^2/Vs	electron mobility	[9]

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After obtaining the optimum thickness of TiO_2 photoanode, the variations in electron diffusion coefficient values were made due to work temperature changes that may occur when DSSC was exposed to the sunlight. Then, the increase in the electron diffusion coefficient value was connected graphically to the voltage value generated by the DSSC, so that the graph (D-V) was obtained. This simulation was conducted by solving the mathematical equations in DSSC, which were the Equation (1) for the value of the electric current, Equation (2) for the voltage, Equation (3) for the efficiency value of DSSC, and Equation (4) for calculating electron diffusion coefficient [9,11]:

$$J_{sc} = \frac{q\phi L\alpha}{1-L^2\alpha^2}\left[-L\alpha + \tanh\left(\frac{d}{L}\right) + \frac{L\alpha\exp(-d\alpha)}{\cosh\left(\frac{d}{L}\right)}\right] \tag{1}$$

$$V_{oc} = \frac{kTm}{q}\ln\left[\frac{L(J_{sc}-J)}{qDn_0\tanh\left(\frac{d}{L}\right)} + 1\right] \tag{2}$$

$$\eta = \frac{P_{max}}{P_{in}} \times 100\% \tag{3}$$

$$D = \frac{kT\mu}{q} \tag{4}$$

3. Results and Discussion

The completion of Equation (1) through Equation (3) in a simulation could produce a relationship between electric current vs. electrical voltage (J-V) and maximum electrical power vs. open voltage (P-V) curves on various TiO_2 thicknesses. The typical results are shown in Figure 1 and Figure 2. The purpose was to obtain the optimum thickness of TiO_2 photoanode because in this state, TiO_2 could properly pass solar light energy into the DSSC. This could be proven by the J_{sc}, V_{oc}, and P_{max} as written in Table 2.

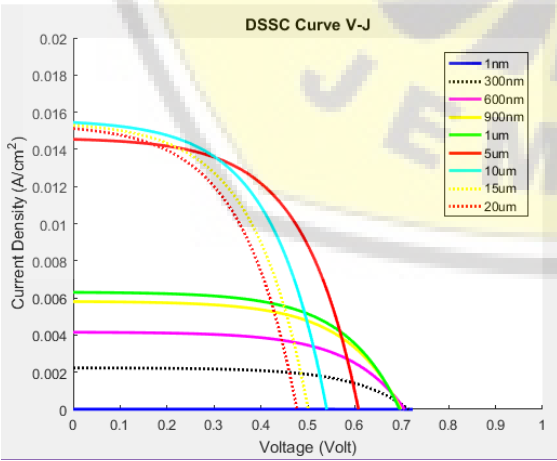

Figure 1. DSSC J-V curve on various thicknesses of TiO_2 photoanode (d)

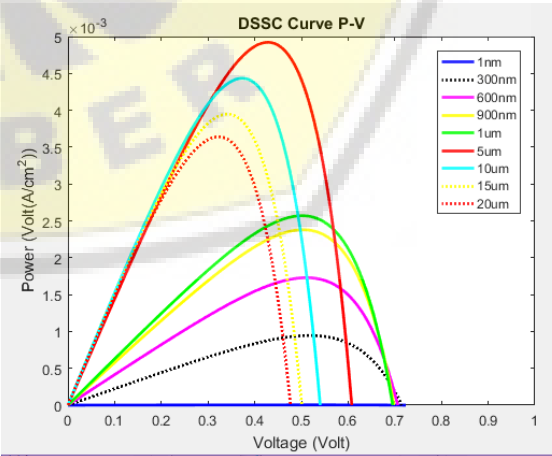

Figure 2. DSSC P-V curve on different thickness variations of TiO_2 photoanode (d)

The determination of the optimum thickness of TiO_2 photoanode was analyzed based on Figure 1, Figure 2, and Table 2. In Figure 1, the optimum current density in the TiO_2 thickness was 5 µm and 10 µm. Meanwhile, Figure 2 is a result showing the maximum power (P_{max}) ascribed by the peaks. The highest was achieved by the sample with the thickness of 5 µm. This can be seen in Table 2, the highest P_{max} was 0.0049 V·A/cm^2.

Table 2. Simulation results at the different thicknesses (d) at 300 K

d	J_{sc} (A/cm^2)	V_{oc} (Volt)	P_{max} (Volt A/cm^2)	η (%)
1 nm	8.0080 x 10^{-6}	0.7234	3.4469 x 10^{-6}	0.0034
300 nm	0.0022	0.7149	0.0009	0.9448
600 nm	0.0042	0.7065	0.0017	1.700
900 nm	0.0058	0.6983	0.0024	2.400
1 µm	0.0063	0.6957	0.0026	2.600
5 µm	0.0145	0.6079	0.0049	4.900
10 µm	0.0154	0.5402	0.0044	4.400
15 µm	0.0153	0.5008	0.0039	3.900
20 µm	0.0151	0.4768	0.0036	3.600

Based on the simulation results, it is shown that the P-V curve was like a parabolic graph due to the occurrence of processes in the DSSC namely the generation of recombination of charge carriers, especially electrons in a certain time span (lifetime). P_{max} is the peak point on the P-V curve which is the limit of the change of electron generation events to recombination. The existence of these events caused an electrical phenomenon when DSSC was exposed to the sunlight. At a thickness of 5 µm, the highest efficiency (η) and increase in the current density (J_{sc}) were obtained. Based on these data, it is known that the thickness of TiO_2 photoanode had an important role in accordance with the research of Ni et al. [11] that the thickness of TiO_2 gave a change in the performance of DSSC.

By obtaining the optimum thickness, we further analyzed other factors such as working temperature associated with the length of time DSSC exposed under the sunlight. By implementing Equation (4), we found that the working temperature affected the electrical parameters in the DSSC namely electron diffusion coefficient (D). By assuming TiO_2 electron mobility was constant of 0.3 cm^2/V.s [17], the working temperature (T) and the electron diffusion coefficient (D) increased as well. This relationship is illustrated in Figure 3.

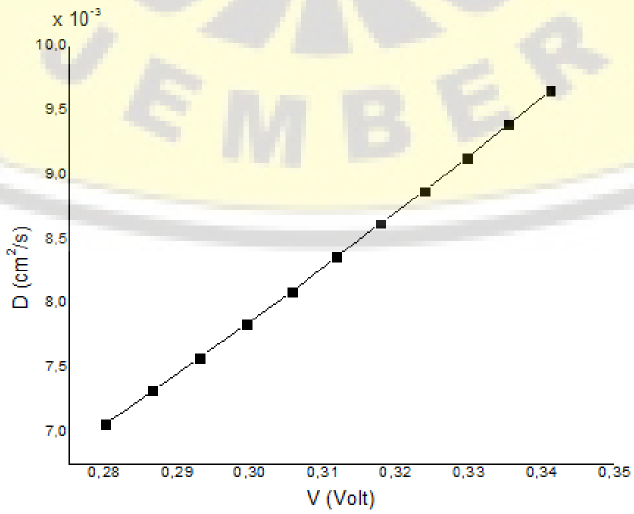

Figure 3. The graph of electron diffusion coefficients vs. voltage of DSSC (D-V) for the sample with a thickness of TiO_2 (5 µm)

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The simulated electron coefficient diffusion (D) was obtained with analytical calculations based on the equation (4) at working temperature of 273 K to 373 K. The DSSC parameters inferred from Figure 3 and Equation (4) are listed in Table 3.

Table 3. Simulation results of electron diffusion coefficient (D) at an optimum thickness (5 μm)

D (cm²/s)	J_{sc} (A/cm²)	V_{oc} (Volt)	P_{max} (Volt A/cm²)	η (%)
7.06 x 10^{-3}	0.0145	0.2800	0.0017	1.700
7.32 x 10^{-3}	0.0145	0.2866	0.0018	1.800
7.58 x 10^{-3}	0.0145	0.2930	0.0018	1.800
7.84 x 10^{-3}	0.0145	0.2994	0.0018	1.800
8.09 x 10^{-3}	0.0145	0.3057	0.0018	1.800
8.36 x 10^{-3}	0.0145	0.3117	0.0019	1.900
8.62 x 10^{-3}	0.0145	0.3178	0.0019	1.900
8.87 x 10^{-3}	0.0145	0.3238	0.0019	1.900
9.13 x 10^{-3}	0.0145	0.3297	0.0020	2.000
9.39 x 10^{-3}	0.0145	0.3354	0.0020	2.000
9.65 x 10^{-3}	0.0145	0.3411	0.0020	2.000

From Table 3, we found that the highest electrical parameter of DSSC was at the most considerable electron diffusion coefficient 9.65×10^{-3} cm²/s. This result is in accordance with the research of Ni *et al.* [11]. Ni *et al.* [11] reported that the changes in the electron diffusion coefficient were strongly affected by the TiO_2 thickness at room temperature (300 K). In the case of DSSC when exposed at a relatively long time, it may cause the working temperature of DSSC to increase more than room temperature (300 K). At the optimum thickness of TiO_2, one of the parameters that change due to the increase in the working temperature of the DSSC is the electron diffusion coefficient. The results obtained from this study are written in Table 3 and Figure 3 showing the greater the working temperature, the greater the electron diffusion coefficient. The electron diffusion coefficient affects the open voltage (V_{oc}), maximum power (P_{max}), and its efficiency (η). An empirical work of various metal oxides may be found in recent works [18,19] and references therein.

On the other hand, the changes of the electron diffusion coefficient do not sufficiently affect the current density (J_{sc}). This result occurred because the J_{sc} is significantly dependent on sunlight intensity on the surface of the DSSC. The intensity of sunlight was assumed to be constant at (100 mW/cm² or 1×10^{17} $cm^{-2}s^{-1}$ corresponds to Table 1. In addition, the difference in the electron diffusion coefficients between the simulated data was quite small due to the weak change in DSSC working temperature [12]. This condition proves that a weak change in the electron diffusion coefficient is not significant effect on the current density of DSSC. Physically, the diffusion coefficient reflects how big the gradient/difference in electron concentration. So, in general, the greater electron diffusion coefficient can affect the voltage generated by DSSC. There are many reports associated with the current study. The trend is closely similar with different optimum and also slightly different features. Several related solar cell parameters could be also considered. A relative rigor inferential work on various solar cell parameter fittings is recently reported [20].

4. Conclusion

By the simulation method, we found that the optimum thickness of TiO_2 DSSC photoanode was 5 μm. At the optimum thickness of TiO_2 photoanode, it was shown that the higher electron diffusion coefficient (D), the open voltage increased V_{oc}. The highest electron diffusion coefficient of 9.65×10^{-3} cm²/s and the working temperature of 373 K produced a maximum power of $P_{max} = 0.0020$ V·A/cm² and open voltage of $V_{oc} = 0.3411$ V.

References

[1] Shahzad U 2015 The Need For Renewable Energy Sources *ITEE J. ISSN Int. J. Inf. Technol. Electr. Eng.* 16–8
[2] Herzog A V., Lipman T E and Kammen D M 2001 Renewable Energy Sources *Encycl. Life …* 1–63
[3] Shiroudi A and Taklimi S R H 2011 Demonstration Project of the Solar Hydrogen Energy System Located on Taleghan-Iran: Technical-Economic Assessments 1158–65
[4] Abdulkadir M 2013 Modeling and Simulation of a Solar Photovoltaic System, Its Dynamics and Transient Characteristics in LABVIEW … *Drive Syst.* … **3** 185–92
[5] Kabir E, Kumar P, Kumar S, Adelodun A A and Kim K H 2018 Solar energy: Potential and future prospects *Renew. Sustain. Energy Rev.* **82** 894–900
[6] Lee K-J, Kim J-H, Kim H-S, Shin D, Yoo D-W and Kim H-J 2012 A Study on a Solar Simulator for Dye Sensitized Solar Cells *Int. J. Photoenergy* **2012** 1–11
[7] Dewi N A, Nurosyid F and Supriyanto A 2016 Pengaruh Ketebalan Elektroda Kerja TiO_2 Transparan terhadap Kinerja Dye Sensitized Solar Cell (DSSC) sebagai Aplikasi Solar Window *Indones. J. Appl. Phys.* **6** 73–8
[8] Ramelan A H, Saputro S, Wahyuningsih S, Khoirunisa A, Supriyanto E and Gareso P L 2015 Synthesis of Anatase and Rutile TiO2 Crystals for High-Performance Dye-Sensitized Solar Cells *Adv. Mater. Res.* **1105** 141–5
[9] Gong J and Sumathy K 2012 A Theoretical Study on Third Generation Photovoltaic Technology : Dye-Sensitized Solar Cells *Mech. Eng.*
[10] Ramelan A H, Wahyuningsih S, Saputro S, Supriyanto E and Hanif Q A 2017 TiO_2 Nanostructure Synthesized by Sol-Gel for Dye Sensitized Solar Cells as Renewable Energy Source *Mater. Sci. Eng.* **176** 1–7
[11] Ni M, Leung M K H and Leung D Y C 2008 Theoretical Modelling of The Electrode Thickness Effect on Maximum Power Point of Dye-Sensitized Solar Cell *Can. J. Chem. Eng.* **86** 35–42
[12] Tayyan A A El 2011 Dye Sensitized Solar Cell: Parameters Calculation and Model Integration *J. Electron Devices* **11** 616–24
[13] Kumari J M K W, Sanjeevadharshini N, Dissanayake M A K L, Senadeera G K R and Thotawatthage C A 2016 The effect of TiO_2 photo anode film thickness on photovoltaic properties of dye-sensitized solar cells *Ceylon J. Sci.* **45** 33
[14] Shah W and Biate R L 2016 Design and Simulation of Solar PV Model Using Matlab/Simulink *Int. J. Sci. Eng. Res. Vol. 7 Issue 3 March-2016 ISSN 2229-5518* **7** 551–4
[15] Aboulouard A, Jouaiti A and Elhadadi B 2017 Modelling and Simulation of the Temperature Effect in Dye Sensitized Solar Cells **9** 94–8
[16] Gong J, Liang J and Sumathy K 2012 Review on dye-sensitized solar cells (DSSCs): Fundamental concepts and novel materials *Renew. Sustain. Energy Rev.* **16** 5848–60
[17] Gong J, Sumathy K, Zhou Z and Qiao Q 2017 Modeling of interfacial and bulk charge transfer in dye-sensitized solar cells *Cogent Eng.* **160** 1–19
[18] Solehudin, Diantoro M, Sa'adah U and Hidayat A 2018 Effect of SnO_2 Nanoparticles on Band Gap Energy of x(SnO_2)-y(Ag)-β-Carotene/FTO Thin Film J. Phys. Conf. Ser. 1093 012049
[19] Sa'adah U, Hidayat A, Solehudin, Sujito, Mufti N and Diantoro M 2018 Band Gap Shift and Electrical Conductivity of (Ag-xSnO_2)NPs-β-Carotene Thin Film J. Phys. Conf. Ser. 1093 012032
[20] Diantoro M, Suprayogi T, Hidayat A, Taufiq A, Fuad A and Suryana R 2018 Shockley's Equation Fit Analyses for Solar Cell Parameters from I-V Curves *Int. J. Photoenergy* **2018** 1–7