Sains Malaysiana 46(3)(2017): 503–508
http://dx.doi.org/10.17576/jsm-2017-4603-19

Applications of Taguchi Method for Optimization of Dye Solar Cell Design

(Aplikasi Kaedah Taguchi untuk Pengoptimuman Reka Bentuk Sel Pewarna Suria)

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ABSTRACT

This paper addresses the optimal Dye Solar Cell (DSC) design considering parameters namely TiO_2 thickness, surface area, iodide concentration in electrolyte and TiO_2 passivation layer thickness as they have influence on DSC performance. It aims to do the research of the practical use of Taguchi method in the optimization of DSC design in order to improve the performance of DSC. This work highlight on the integration of Taguchi method with simulation which showed that the optimal design of DSC is 10 μm thickness of TiO_2, 90m^2/g of TiO_2 photoelectrode surface area, 1 M iodide concentration in electrolyte and two layers with 20 nm thickness of TiO_2 passivation layer with efficiency of 4.59165%. All the features of the Taguchi-based optimization were also discussed.

Keywords: Dye solar cell; efficiency; passivation layer; Taguchi Method; TiO_2

ABSTRAK

Kertas ini membincangkan tentang reka bentuk sel suria pewarna (DSC) optimal yang mengambil kira parameter seperti ketebalan TiO_2, kawasan permukaan, kepekatan iodida dalam elektrolit dan ketebalan lapisan pempasifan TiO_2 kerana ia mempengaruhi prestasi DSC. Tujuannya ialah untuk menjalankan penyelidikan tentang penggunaan kaedah Taguchi secara praktikal dalam pengoptimuman reka bentuk DSC untuk meningkatkan prestasi DSC. Kertas ini tertumpu kepada integrasi kaedah Taguchi dengan simulasi yang menunjukkan pengoptimuman reka bentuk DSC ialah ketebalan 10 μm TiO_2, 90 m^2/g TiO_2 kawasan permukaan fotoelektrod, 1 M kepekatan iodida dalam elektrolit dan dua lapisan ketebalan 20 nm TiO_2 lapisan pempasifan dengan kecekapan 4.59165%. Semua sifat pengoptimuman berasaskan Taguchi juga dibincangkan.

Kata kunci: Kaedah Taguchi; lapisan pempasifan; kecekapan; sel pewarna suria; TiO_2

INTRODUCTION

Dye Solar Cell (DSC) belongs to the third generation of solar cell that offers eco-friendly, low cost and simple fabrication procedure (Graetzel 2003). DSC consists of sandwich like structure of dye-sensitized TiO_2 layer, electrolyte and counter electrode between transparent conducting oxide (TCO) glasses. Components used for build the DSC is nontoxic material and also huge in amount in the world. The procedure to build the DSC is easy. However, there are lots of problem that still may need to be addressed in DSC. One of them is its still low efficiency. The optimal performance of DSC usually presented in efficiency along with (1),

$$Efficiency = \frac{J_{sc}V_{oc}FF}{I_s} \quad (1)$$

where J_{sc} is the current density when short current condition (A/m^2); V_{oc} is the voltage when open circuit condition (V); FF is fill factor; and I_s is incident source light (W/m^2).

Several things affect the efficiency of DSC such as resistance and recombination. Higher resistance may reduce the mobility of electron inside the DSC. Low mobility of electron may result in low J_{sc} of DSC. According to (1), low J_{sc} will bring DSC to low efficiency. Meanwhile, recombination occurs when the electron do the back reaction to the redox electrolyte or hole mediator in DSC (Adachi et al. 2006). It may cause significant losses in V_{oc} of DSC. Moreover, high recombination will add another resistance on electron mobility. It can be said that low resistances and recombination can produce higher J_{sc} and V_{oc} as well as efficiency of DSC. In order to improve the performance of DSC, reducing the resistance and recombination is important.

It has been reported on previous works that several components affect the performance of DSC. One of them is the resistance influenced by thickness of TiO_2 as photoelectrode in DSC (Zhang et al. 2010). Thicker layer of TiO_2 will enhance the amount of dye absorbed as well as captured energy from the sun but also higher transport resistance which limits the mobility of electron inside DSC. Another component that impacts DSC performance is electrolyte concentration used in DSC. Higher electrolyte concentration may increase the electron diffusion but on the other hand, electron lifetime will get lower (Zhang et al. 2009). Higher electron diffusion means electron can move easier in DSC. Higher electron lifetime brings electron may stay longer in DSC. Those conditions can improve J_{sc} of DSC. Next component brings effect to the performance of DSC is the surface area of photoelectrode used. Larger surface area of TiO_2 has benefit in light scattering conversely lack of mobility. Passivation layer used in DSC also makes impression on the performance of DSC. By adding passivation layer of TiO_2 may help in reducing the recombination which is mainly at the TCO/electrolyte interface and at the photoelectrode film/electrolyte interface (Caramori et al. 2010; Hossain et al. 2008; Jin et al. 2012). Those conditions highpoint the prospective of employing optimized components of DSC to reach its optimum performance.

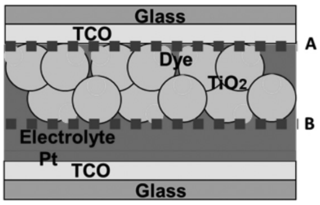

FIGURE 1. DSC Model

In this paper, experiment of DSC model as shown in Figure 1 using such optimum DSC components namely thickness of TiO_2, iodide concentration in electrolyte, surface area of TiO_2 morphology and adding TiO_2 passivation layer. Works are conducted based on Taguchi method. It can be helpful for further research since experimental works need more cost to be conducted than simulation.

METHODS

EXPERIMENT SETUP

Simulations of DSC are executed using ATHENA and ATLAS by Silvaco. Semiconductor fabrication design, device and process in automation technologies can be built in ATHENA. By using ATLAS, research can be assisted in simulating electrical behavior of semiconductor devices including solar cell. Michael et al. (2005) reported that simulation work of solar cell can use ATLAS as its modelling software. In ATHENA, there are several models offered. Shockley-Read-Hall (SRH) model is the closest model to represent DSC. SRH model showed mechanism of electron transport of wide band gap semiconductor where TiO_2 belongs. It also defines kinetics of generation-recombination process within semiconductor, not only on interface. SRH model also be used for research by Goudon et al. (2007).

Simulation may represent costly experimental works. Simulation can propose design for fabrication even though others factor influence in practice. For the input of simulation, properties of TiO_2 namely affinity, energy gap and permittivity are captured from literatures. Data properties used in simulation are as shown in Table 1. According to those data properties, DSC is modelled in ATHENA with active area of 1 cm^2 using N719 dye.

TABLE 1. TiO_2 properties

Property	Unit	Value	Ref.
Affinity	eV	4.3	(Fuke et al. 2009)
Energy gap	eV	3.2	(Graetzel 2003)
Permittivity	F/cm	46	(Patil et al. 2009)

TAGUCHI-BASED DESIGN

Taguchi methods (Taguchi 1990) have been widely used in engineering analysis and plan experiments with the objective of obtaining data in an organized way about specific condition. The benefits of this method is the saving effort to do experiments; saving experimental time, reducing the cost and investigating involved significant factors easier.

With calculating the signal – to – noise (S/N) ratio, a statistical analysis of variance (ANOVA) can be done to investigate the impact of some DSC parameters on its efficiency. The steps applied for Taguchi optimization in this work are select control factors, select Taguchi orthogonal array, conduct experiments, DSC efficiency measurement, analyse results, predict optimum DSC performance and confirmation experiment.

Taguchi's model offers several arrays to be used. It can be chosen based on appropriate experiment's requirement. One of Taguchi's model arrays is L8 as shown in Figure 2. This array can be used for experiment with up to seven involved factors with two levels for each factor. It is chosen for the work in this paper because experiment considers

FIGURE 2. Taguchi's model L8 orthogonal array

No.	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6	Factor 7
1	1	1	1	1	1	1	1
2	1	1	1	2	2	2	2
3	1	2	2	1	1	2	2
4	1	2	2	2	2	1	1
5	2	1	2	1	2	1	2
6	2	1	2	2	1	2	1
7	2	2	1	1	2	2	1
8	2	2	1	2	1	1	2

five factors. The effects of different thickness of TiO_2, structure of TiO_2, iodide concentration in electrolyte and adding TiO_2 passivation layer on DSC structure will be varied to get the optimum performance of DSC. Eight different designs are then simulated based on the Taguchi's model L8 array.

Taguchi method focuses on the significance of evaluating the S/N ratio. It is in order to minimize variations in experiment design due to uncontrollable parameter. In this work, the higher efficiency represents better performance of DSC. Because of that reason, the DSC efficiency was considered as the quality characteristic with the concept of 'the larger-the-better'. The S/N ratio for the larger-the-better is as shown in (2),

$$S/N = -10log\left(\frac{1}{n}\sum_{i=1}^{n}\frac{1}{y^2}\right), \tag{2}$$

where n is the number of measurements in an experiment, in this case, n=1 and y is the measured efficiency value in an experiment. The S/N ratio values in this work are calculated by considering equation (2). Since greater S/N value resembles to a better performance of DSC, the optimal level of the DSC parameters is the level with the greatest S/N value.

The degrees of freedom for five parameters in each of two levels were calculated as in (3).

Degree of Freedom (DOF) = number of levels -1. (3)

For each factor in this work, DOF equal to: DOF = 2 – 1 = 1. Since L8 OA is used, it has eight DOF, in which 6 were assigned to three factors where each one has 2 DOF and 2 DOF was assigned to the error. For the purpose of detecting the degree of influence of the DSC parameters on its efficiency, five factors, each at two levels, are taken into account, as shown in Table 2.

The value chosen as levels 1 and 2 are the optimum values based on previous study. The thicknesses of TiO_2 used in DSC are 10 and 12 μm (Oktiawati et al. 2013). The iodide concentrations in electrolyte occupied in DSC are 0.5 and 1 M (Oktiawati et al. 2014). The TiO_2 passivation layers are at TCO/electrolyte interface as indicated as passivation layer A in Figure 1 and at the TiO_2 photoelectrode film/electrolyte interface as indicated as passivation layer B in Figure 1 with thickness of 20 nm for each TiO_2 passivation layer (Eskandar et al. 2012; Mohamed et al. 2015). The surface areas of TiO_2 photoelectrode are 50 m^2/g as representation of TiO_2 nanoparticle commonly used in DSC and 90 m^2/g for different size of TiO_2 nanoparticle (Shanmugam et al. 2009; Waita et al. 2007).

ANOVA

After conducting calculation of efficiency and S/N ratio for each condition as designed, ANOVA is also carried out. ANOVA is a statistically based tool for distinguishing any differences in the typical performance of groups of parameters as factor tested. ANOVA aids in analysis the impact of all factors and their relations by comparing the mean square with an approximation of the experimental errors at specific levels.

Statistically, there is also a tool called an F test to see which design factors have a significant influence on the feature representative. In the analysis, the F-ratio is a ratio of the mean square error to the residual error, and is traditionally used to determine the implication of a factor. The P-value reports the impact level which one is suitable and unsuitable to be used later on.

RESULTS AND DISCUSSION

TAGUCHI METHOD APPLICATION

S/N Ratio Results Eight experiments were conducted at different setup of five parameters coded based on L8 OA design. The DSC efficiency measured from the experiments with Taguchi method application and their corresponding S/N ratio values are listed in Table 3.

From Table 3, it can be seen that experiment 4 with condition of 10 μm of TiO_2 thickness, 1 M of iodide concentration in electrolyte, 20 nm thickness of TiO_2 passivation layer A, 20 nm thickness of TiO_2 passivation layer B and surface area of 90 m^2/g for TiO_2 as photoelectrode showed the higher efficiency of DSC among others which is 4.59165% and has the S/N ratio of 13.23938, respectively.

The S/N ratio values by factor level response table for DSC parameters namely the TiO_2 thickness, iodide concentration in electrolyte, thickness of TiO_2 passivation layer A, thickness of TiO_2 passivation layer B and surface area of TiO_2 as photoelectrode was listed and the delta results are given in Table 4.

Based on the analysis of the S/N ratio value for DSC parameters by factor level, the highest delta is the top rank.

TABLE 2. Parameters of DSC design

Parameter	Unit	code	Level 1	Level 2
TiO_2 thickness	μm	A	10	12
Iodide concentration	M	B	0.5	1
Passivation layer A	nm	C	0	20
Passivation layer B	nm	D	0	20
Surface area	m^2/g	E	50	90

TABLE 3. Experiment results

No	A	B	C	D	E	Efficiency	S/N ratio
1	10	0.5	0	0	50	3.60355	11.13461
2	10	0.5	0	20	90	4.27342	12.61551
3	10	1	20	0	50	4.49532	13.05521
4	10	1	20	20	90	4.59165	13.23938
5	12	0.5	20	0	90	4.40566	12.88022
6	12	0.5	20	20	50	4.22973	12.52625
7	12	1	0	0	90	3.88505	11.78793
8	12	1	0	20	50	3.88321	11.78382

On the other hand, as shown in Table 4, the optimal DSC performance was obtained with 10 µm of TiO_2 thickness (level 1), 1 M of iodide concentration in electrolyte (level 2), 20 nm thickness of TiO_2 passivation layer A (level 2), 20 nm thickness of TiO_2 passivation layer B (level 2) and 90 m^2/g for surface area of TiO_2 photoelectrode (level 2) with value of S/N ratio are 12.51118, 12.46658, 12.92527, 12.54124 and 12.63076, respectively. It also shows that the list of factors from the most to the less impactful parameters to the DSC efficiency is TiO_2 passivation layer A, surface area of TiO_2 photoelectrode, TiO_2 passivation layer B, TiO_2 thickness and iodide concentration in electrolyte as shown as rank in Table 4.

For further analysis, the TiO_2 thickness, iodide concentration in electrolyte, TiO_2 passivation layer A, TiO_2 passivation layer B and surface area of TiO_2 photoelectrode were considered in the mathematical models for DSC efficiency. The correlation between those five factors and DSC efficiency were obtained by multiple linear regressions. The standard commercial statistical software package in EXCEL was used to derive the models of the form as shown as (4).

$$\text{Efficiency} = -0.07003625A + 0.171435B + 0.025964125C + 0.007355375D + 0.005899813E \quad (4)$$

From (4), it can be seen that the DSC efficiency is directly proportional with the iodide concentration in electrolyte as factor B, thickness of TiO_2 passivation layer A as factor C, thickness of TiO_2 passivation layer B as factor D and surface area of TiO_2 photoelectrode as factor E, also inversely proportional with TiO_2 thickness as factor A. Moreover, in multiple linear regression analysis, there is a value of R^2 which is the regression coefficient where R^2 is 0.892788 for the models, which indicate that the fit of the experimental data is satisfactory.

ANOVA Results The ANOVA results for this work are illustrated in Table 5. The percentage numbers represent that those DSC parameters have significant effects on DSC efficiency. It can be seen from Table 5 that the TiO_2 thickness, iodide concentration in electrolyte, thickness of TiO_2 passivation layer A, thickness of TiO_2 passivation layer B and TiO_2 photoelectrode surface area affect the DSC efficiency by 3.856396%, 1.707934%, 65.02146%, 5.79174% and 13.8779% respectively. From those results, it showed that the presence of TiO_2 passivation layer at TCO/electrolyte interface as indicated as passivation layer A in Figure 1 is so impactful to enhance the efficiency of DSC. Another important parameter that is also impactful to improve the efficiency of DSC is the TiO_2 photoelectrode surface area. It can be seen from the result that larger surface area of TiO_2 photoelectrode used may improve the efficiency of DSC. One of the ways to get larger surface area of TiO_2 photoelectrode is occupying particle with smaller size or using composite paste of common nanoparticle with bigger particles as DSC photoelectrode. A confirmation for this experiment design is necessary in order to verify the optimum conditions of DSC design.

CONFIRMATION DESIGN

The experimental confirmation is the final stage in validating the results based on Taguchi's design approach. The confirmation experiment is a crucial step and is highly recommended by Taguchi to verify the experimental result. The optimal conditions are set for the significant factors namely TiO_2 thickness, iodide concentration in electrolyte,

TABLE 4. S/N ratio values for DSC parameters by factor level

Level	TiO_2 thickness	Iodide conc	Pass layer A	Pass layer B	Surface Area
1	**12.51118**	12.28915	11.83047	12.21449	12.12497
2	12.24456	**12.46658**	**12.92527**	**12.54124**	**12.63076**
delta	0.266622	0.177436	1.094797	0.326746	0.505786
rank	4	5	1	3	2

TABLE 5. ANOVA results

Source of Variation	DOF	SS	Var	F ratio	P value	%
A. TiO_2 thickness	1	0.035544	0.017772	0.395748	0.448581	3.856396
B. Iodide concentration	1	0.015742	0.007871	0.17527	0.62502	1.707934
C. Pass layer A	1	0.59929	0.299645	6.67258	0.074128	**65.02146**
D. Pass layer B	1	0.053381	0.026691	0.594355	0.429745	5.79174
E. Surface Area	1	0.12791	0.063955	1.424166	0.255953	13.8779
Error	1	0.089814	0.044907			9.744575
Total	6	0.921681				100

thickness of TiO_2 passivation layer A, thickness of TiO_2 passivation layer B and TiO_2 photoelectrode surface area while the insignificant factors are set at economic levels such as N719 dye, 1 cm^2 active area, Pt as counter electrode and a selected number of experiments are run under defined conditions. The result from the confirmation experiment is compared with the predicted based on the parameters and levels tested. In this study, a confirmation experiment was conducted by utilizing the appropriate level of the optimal DSC parameters (A1B2C2D2E2) for DSC efficiency and obtained as 4.59165% as shown in Table 3 as experiment no. 4.

The DSC efficiency increases with thick enough layer of TiO_2 so DSC has enough amount of dye to absorb energy from the sun. Thick enough layer of TiO_2 also has not so high enough transport resistance as well as high mobility of electron inside DSC. It is agreed with the work by Unan Yusmaniar et al. (2013) showed that the optimum thickness of TiO_2 used in DSC as photoelectrode is 10 μm. Enough iodide concentration in electrolyte increases the electron diffusion. On the other hand, its electron lifetime will not be too low so it can contribute in enhancing DSC efficiency. Work by Zhang et al. (2009) reported that DSC with iodide concentration more than 1 M in electrolyte could not improve DSC performance anymore. Larger morphology of TiO_2 as photoelectrode used in DSC has benefit in light scattering but conversely it has lack of mobility. Therefore, composite TiO_2 paste as photoelectrode of small and large particles is proposed to be occupied. Adding passivation layer of TiO_2 may help in reducing the recombination which is mainly happen at the TCO/electrolyte interface as mentioned as passivation layer A than at the TiO_2 photoelectrode film/electrolyte interface as indicated as passivation layer B in Figure 1. Experimental work proved that DSC with additional layer of TiO_2 as passivation layer at the TCO/electrolyte interface and at the TiO_2 photoelectrode film/electrolyte interface showed better efficiency than DSC without passivation layer (Mohamed et al. 2015).

Conclusion

A research in the optimization of dye solar cell based on Taguchi method has been discussed. The proposed design shows that the optimum DSC efficiency of 4.59165% can be reached by utilizing 10 μm thickness of TiO_2, 90 m^2/g of surface area for TiO_2 photoelectrode which can be made by occupying smaller size of particle used as photoelectrode or composite TiO_2 paste as photoelectrode of small and large particles, 1 M iodide concentration in electrolyte and adding 20 nm thickness of TiO_2 passivation layer at TCO/electrolyte interface and at the TiO_2 photoelectrode film/electrolyte interface.

Acknowledgements

The authors gratefully acknowledge the support from Centre of Innovative Nanostructures & Nanodevices (COINN) and Graduate Assistant Scheme by Universiti Teknologi Petronas, Perak, Malaysia.

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Received: 17 Disember 2015
Accepted: 14 September 2016