Dye-sensitized solar cell simulation performance using MATLAB

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Abstract. In this paper, we analyzed J-V curve of the Dye-Sensitized Solar Cell (DSSC) using numerical calculations. The simulation is based on differential equation of photoelectrochemical in the DSSC. Using internal parameters of the DSSC (L, D, n₀, t) appropriate for TiO₂, we calculate the J-V curve numerically. The analysis is performed by also making variations in temperature, irradiant, absorption constant and photoelectrode thickness. We found that irradiant affect the J-V curve significantly compared to the three other variables. The change in absorption constant needs to be in a factor at least in order of 100 or more to obtain a change, which is considerably high in J-V curve. It is also found that the thickness of photoelectrode should be carefully considered since very thin thickness cannot support DSSC process.

Keywords: DSSC, photovoltaic, simulation performance, temperature, layer thickness

1. Introduction

Since it has many advantages such as environmental friendly, cheap and easy to produce, Dye-Sensitized Solar Cell (DSSC) attracts many attentions in the last two decades [1-8]. It had also been reported that DSSC was able to reach energy efficiency above 10% [9]. DSSC is generally comprised of two electrodes, which act as a photoelectrode and an inverting electrode. The photoelectrode is usually made from semiconductor material (TiO₂ or ZnO) deposited on conductive transparent conductive (TCO) glass which is sensitized to ruthenium dye. The second electrode, which is an inverting electrode, is formed from Pt deposited on TCO glass. Then, the electrolyte iodide / triiodide (I⁻ / I₃⁻) is sandwiched between these electrodes [10-11].

The injection of the dye molecules leads to the formation of the electrons which then flow on the photoelectrode from a thin layer of porous semiconductor to the TCO. In this condition, there is a smoothing of the trap that depends on the intensity of injection. The oxidized dye molecules are regenerated by a redox (reduction-oxidation) mediator. Then, this oxidized redox mediator is transported to the inverting electrode where it regenerates for complete DSSC distribution. Due to the very small size of the semiconductor particles and the strong electrolyte filtering effect, the value of the macroscopic electric field is not significant. Thus, the electrons and the redox medium are transported by the diffusion process [12-13].
The injected electrons due to the photon intensities with wavelength related to the color of the dye material will be excited to the semiconductor conduction band. This lead to the increase of the electron density in the thin layer of the porous electrode, result in the shifting of the quasi-Fermi level close to the conduction band gap $E_c$. Theoretically, the difference between semiconductor Fermi level $E_F$ and the electrolyte redox potential ($E_{\text{redox}}$) is assumed to be induced photovoltaic [13-16]. In the end, there will be an open circuit condition where no current flows through the photoelectrode interface and the electrolyte/inverting electrode interface. However, under maximum power conditions, the potential difference will increase between the two interfaces on the DSSC.

In this paper, we study the performance of DSSC by analyzing J-V curve in various condition. In numerical calculation, we use parameters represents semiconductor material-based DSSC. This research modeled the theory on DSSC with diffusion diffraction model for it is parameter effect on J-V image which will be discussed in this article.

2. Methods

This research was initiated from references and related data computing DSSC. After obtaining the equations of the existing references, modeled into a software program based on MATLAB. Then add the values used as internal parameters DSSC into MATLAB programming. The modeling was to simulate the performance curve J-V in DSSC.

In 1994, Sven Södergren et al. analyzed theoretically the photoelectrochemical behavior in the DSSC photoelectrode nanostructure. The resulted equation relates the electron transport, electron recombination, and electron photogeneration in thin films DSSC as [13]

$$D \frac{\partial^2 n(x)}{\partial x^2} - \frac{n(x) - n_o}{\tau} + \phi_o \alpha \exp(-\alpha x) = \frac{\partial n}{\partial t} \quad (1)$$

where $n(x)$ is the number of excessive electron photogeneration concentrations at position $x$ in the photoelectrode interface layer, $n_o$ represents concentration of electrons below the equilibrium of the dark conditions, $D$ correspond to the diffusion coefficient of the electron. The parameters $\tau$, $\phi_o$ and $\alpha$ represent the lifetime of the free electrons in the conduction band, the intensity Flux illumination of photons and light absorption coefficient of the thin film. In the steady state of the DSSC irradiation, equation (1) becomes

$$D \frac{\partial^2 n(x)}{\partial x^2} - \frac{n(x) - n_o}{\tau} + \phi_o \alpha \exp(-\alpha x) = 0. \quad (2)$$

In a short circuit state, the electron is easily extracted as a current and there is no electron flowing directly to the inverting electrode. Therefore, the two required boundary conditions are

$$n(0) = n_o \quad (3)$$

and

$$\frac{dn}{dx}\big|_{x=d} = 0 \quad (4)$$

where $d$ represents the thickness of the porous photoelectrode layer. In order to complete the DSSC model, the excessive amount of electron concentration from the photogeneration process at the contact (n-contact) is considered in the photovoltaic value ($V_{ph}$) as [13,17]

$$V_{ph} = \frac{kT}{q} \ln \frac{n_{\text{contact}}}{n_o} \quad (5)$$

The current density in a short circuit condition ($J_{sc}$) is determined by the equation such [13,17]
where \( L = \sqrt{D\tau} \) is the length of electron diffusion. We assume that DSSC works on the potential difference \( V \) between the Fermi level of the photoelectrode and the redox potential of the electrolyte, then the density value of the excessive electron at the photoelectrode interface \((x = 0)\) increases and the value of \( n \) becomes a state with \( n(0) = n_0 \). Based on equations (2) and (5), the relationship between current density and the voltage can be illustrated by an equation such [13,17]

\[
J = J_{sc} - \frac{q\Phi n_0}{L} \tanh \left( \frac{qV}{kT} \right) \left[ \exp \left( \frac{qV}{kT} \right) - 1 \right]
\]  

(7)

while the voltage is determined as

\[
V = \frac{kT}{q} \ln \left[ \frac{L(J_{sc} - \overline{J})}{qdn_0 \tanh \left( \frac{qV}{kT} \right)} \right]
\]  

(8)

where \( q \) is the charge of electrons, \( d \) represents the thickness in the thin layer of DSSC, \( m \) is associated with the ideal factor, \( T \) is the absolute temperature, and \( k \) is the Boltzmann constant. The \( J-V \) curve can be easily derived from Equation(7). This curve is commonly used in \( J-V \) meter characterization to determine the efficiency value of solar cells. In this paper, we use internal parameters in the DSSC (\( \Phi, \alpha, m, L, D \)) from previous researches which are written in table1.

### Table 1. The published value of DSSC internal parameters and factors.

| Parameters | Published value |
|------------|-----------------|
| \( L \) (cm\(^1\)s\(^{-1}\)) | \(2.2361 \times 10^{-3}\) Refs. [23] |
| \( \alpha \) (cm\(^{-1}\)) | 5000 Refs. [14,17,18,22] |
| \( m \) | 4.5 Refs. [13,17,18,22] |
| \( D \) (cm\(^1\)s\(^{-1}\)) | \(5.0 \times 10^{-4}\)Refs. [17,22] |
| \( n_0 \) | \(10^{16}\)Refs. [17, 19, 20,22] |
| \( \tau \) (ms) | 10 Refs. [14, 17, 21,22] |
| \( \Phi \) (cm\(^2\)s\(^{-1}\)) | \(1.0 \times 10^{17}\)Refs. [14,17,18,22] |
| \( d \) (cm) | \(10 \times 10^{-4}\)Refs. [21,22,23] |
| \( T \) (K) | 300 Refs. [21,22,23] |

A good relation between the characteristics of J-V can yield a graphical curve corresponding to the calculations and experiments performed in accordance with figure1.
Figure 1. J-V Characteristic based in data [18]

3. Results and Discussion
In this study, we analyze the effect of several variations, i.e.: temperature ($T$), the intensity of irradiation ($\Phi$), the absorption coefficient ($\alpha$) and the thickness of the layer ($d$) on the characteristic of J-V curve. The analysis is performed based on equation 2 which generally describes the DSSC photoelectrochemical behavior. The result of the effect of temperature variation on J-V curve is illustrated in Figure 2. The temperature variation is 273 K (red line), 300 K (green line) and 320 K (blue line). It can be seen that the increase on temperature is rising the J-V curve. It can be seen that the initial voltages are the same for the three variations of temperature. According to the equation (7), the excess of photoelectron does not depend on the temperature. However, the dynamics of the electron is affected by thermal energy, hence the density current is rising by the increase on temperature. We also notice that the temperature variation does not affect the excessive concentration of the electron photogeneration.

Figure 2. J-V Characteristic with temperature variations.
According to Figure 3, the increase of the intensity of the irradiant photon affect the J-V curve significantly. The irradiate variation is $1.0 \times 10^{17}\text{cm}^{-2}\text{s}^{-1}$ (red line), $2.0 \times 10^{17}\text{cm}^{-2}\text{s}^{-1}$ (green line), and $3.0 \times 10^{17}\text{cm}^{-2}\text{s}^{-1}$ (blue line). The increase of irradiance leads to the enhance of the number of the excess electron. Consequently, this increment will also increase the voltage of the photoelectrode and the density of current. This can be predicted using equation (7) and (8).

![Figure 3. J-V Characteristic with irradiation variations](image1)

In the variation of absorption coefficient with the absorption variation is $6000\text{cm}^{-1}$ (red line), $5000\text{cm}^{-1}$ (green line), and $4000\text{cm}^{-1}$ (blue line) as it is illustrated in Figure 4, we found that the effect on J-V curve is not significant. This can be understood since in the absorption process is usually exponential of the absorption coefficient. Hence, to be able to obtain significant change of the excess of photoelectron, it is required the change of the absorption constant is in the order of 1000 times or more. It means that we need to modify the photoelectrode (in example, by depositing the other atom or molecule) to obtain a large absorption constant.

![Figure 4. J-V Characteristic with the variation of absorption constant](image2)
In the thickness of photoelectrode with variation is 4 $\mu$m (red line), 5$\mu$m (green line), and 6$\mu$m (blue line) as it is illustrated in Figure 5, the effect to the J-V curve is relatively small. It is also noticed that in the thickness as thin as 4 $\mu$m, the photoelectrode cannot support the photogeneration process since there is no density current appear. We predict that in this such very thin film there is a short which prevent the process of current generation.

**Figure 5. J-V Characteristic with the variation of the thickness of photoelectrode**

The change in the J-V characteristic curve where the current density of $J_{sc}$ will increase as the maximum power increases due to the increasing thickness of the thin film on the photoelectrode. This process occurs because of the ability of a thick photoelectrode which is able to absorb more photons to a certain extent. Then, there is a decrease due to the photogeneration process that occurs. However, the resulting open $V_{oc}$ circuit voltage does not affect the photoelectrode temperature, so the density value of the current is the same. This occurs because of the electron dilution effect [14]. When the light is transmitted through the pores of the electrode, the intensity slowly falls.

Based on this modelling, there are several things need to be considered in order to produce optimum efficiency value. This can be obtained by choosing the semiconductor material, the thickness of the photoelectrode and the particle size in the material. Thus, simulating the DSSC process is important to achieve better performance in the real experiments.

**4. Conclusion**

This modeling simulation is performed to predict performance on DSSC through the theoretical approach based on internal parameters and factors that make DSSC performance better. This approach is based on analyzing photoelectrochemical behavior on DSSC based on photoelectrode electron diffusion process so that the value of current density of $J_{sc}$ short circuit, $V_{oc}$ open circuit voltage, and maximum point at current and voltage density value of $J_{mp}$ and $V_{mp}$ are obtained. The analysis was performed based on the factors influenceing temperature, irradiation intensity, absorption coefficient, and photoelectrode thickness in DSSC. This study still needs further development by adding the existing parameters as well as external factors to the DSSC to match the experiments performed.
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