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A simple method for modeling dye-sensitized solar cells

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ABSTRACT

Dye-sensitized solar cells (DSCs) are photoelectrochemical photovoltaics based on complicated electrochemical reactions. The modeling and simulation of DSCs are powerful tools for evaluating the performance of DSCs according to a range of factors. Many theoretical methods are used to simulate DSCs. On the other hand, these methods are quite complicated because they are based on a difficult mathematical formula. Therefore, this paper suggests a simple and accurate method for the modeling and simulation of DSCs without complications. The suggested simulation method is based on extracting the coefficient from representative cells and a simple interpolation method. This simulation method was implemented using the power electronic simulation program and C-programming language. The performance of DSCs according to the TiO_2 thickness was simulated, and the simulated results were compared with the experimental data to confirm the accuracy of this simulation method. The suggested modeling strategy derived the accurate current–voltage characteristics of the DSCs according to the TiO_2 thickness with good agreement between the simulation and the experimental results.

1. Introduction

Dye-sensitized solar cells (DSCs) have attracted considerable attention as a low cost and highly efficient solar cell over the last two decades since they were invented by Michael Gratzel and co-workers in 1991 [1]. Unlike conventional *p–n* junction silicon solar cells, DSCs are photoelectrochemical solar cells consisting of a photo-electrode, counter-electrode and electrolyte layer. The cell has a nanoporous semiconductor structure (TiO_2, ZnO, etc.) with dye molecules adsorbed on the photo-electrode, while there is a thin catalytic layer (Pt) for the redox reaction at the counter-electrode. When a DSC is irradiated with sunlight, electrons are generated from the excited dye molecules in the photo-electrode and are injected into the nanoporous semiconductor structure. Consequently, electrons are transferred to an external circuit through the transparent conductive oxide. The excited dye molecules are regenerated by iodide ions in the electrolyte, which is in turn regenerated by the electrons at the counter-electrode [2–4].

The performance of DSCs is determined by a range of factors, such as the light-harvesting ability of the photo-electrode, electron separation in the photo-electrode, electron recombination during the electron transport, catalytic ability of the counter-electrode and the performance of the electrolyte. Therefore, it is essential to optimize these factors for highly efficient DSCs. The modeling and the simulation of DSCs are powerful tools for examining the effect of these factors on the performance of DSCs. The factors can be easily optimized predicting the performance of DSC according to different factors without many repetitive experiments. In addition, the performance of large-scaled DSC modules and power conversion systems for the DSCs can be verified before the installation of DSCs to real-life applications. Therefore, the accurate modeling and simulation of DSCs is valuable for DSC research to reduce the number of time-consuming and trial-and-error experiments.

Several groups have developed a theoretical model for the accurate modeling and simulation of DSCs. Villanueva et al. [5,6] developed a numerical model based on the continuity equation for electrons with a diffusion and recombination constant. Labat et al. [7] suggested the simulation protocol based on a unique density functional theory model for DSCs. Gagliardi et al. [8] implemented a finite element model including the dynamic and continuity equations for electrons in TiO_2, iodide/triiodide ions in the electrolyte and cation. Andrade et al. [9] developed a transient phenomological model for DSCs using the Butler–Volmer equation, dimensionless equation and boundary conditions. These theoretical models for DSCs show the accurate simulation results depending on the different factors. The simulation results from these theoretical models showed good agreement with the experimental results. On the other hand, these models are quite complicated because they are based on complicated mathematical formulae representing the

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chemical reactions in the DSC. Therefore, it is inconvenient to understand the simulation method and time consuming to simulate DSCs.

In this study, a simple and accurate method for the modeling and simulation of DSCs without complicated mathematical formulae is suggested to overcome the disadvantages of the previous simulation method. This simulation method is based on extracting the coefficient from the representative experimental open circuit voltage (V_{OC}) and current density (J_{SC}) data according to the variables as well as a simple interpolation method. This method was implemented using a power electronic simulation program based on the C-programming language. The simulation was carried out by selecting the TiO_2 thickness of the photo-electrode as a variable. Therefore, the simulation revealed the performance of the DSCs according to the TiO_2 thickness. Finally, to test the accuracy of the suggested simulation method in this work, the simulation results were compared with the experimental performance of a DSC according to the TiO_2 thickness.

2. Experiments

Single cells with an active area of 0.25 cm^2 were fabricated to extract the voltage and current coefficient according to the TiO_2 thickness and to obtain the standard current–voltage (*I–V*) characteristics for the simulation of DSCs. The DSCs with TiO_2 thicknesses of 3, 8, 12, 20 and 26 μm were selected as representative cells to extract the coefficients, whereas DSCs with a TiO_2 thickness of 6 μm was selected as the standard cell to obtain the standard *I–V* characteristics. Commercial TiO_2 paste (Ti-Nanoxide HT/SP, Solaronix, Switzerland) was deposited on a cleaned fluorine-doped tin oxide (FTO, 13 Ω/sq; Hartford Glass Co. Inc., USA) substrate by screen printing to fabricate the photo-electrode. The TiO_2 thickness was controlled by the number of screen printing and drying processes at 120 °C for 30 min. The nanoporous TiO_2 structure was completed by sintering at 450 °C for 30 min. After sintering, the photo-electrodes were soaked in a 0.2-mM N719 (*cis-bis*(isothiocyanato) *bis*(2,2′-bipyridyl-4,4′-discarboxylato)–ruthenium(II)–*bis* tertabutyl–ammonium, $RuC_{58}H_{86}N_8O_8S_2$) dye solution for 24 h at room temperature to allow the dye molecules to attach to the nanoporous TiO_2 structure. The dye-sensitized TiO_2 photo-electrode was completed by rinsing with an ethanol solution to remove the excessive dye molecules.

A pre-drilled FTO glass with two pin holes for injecting the electrolyte was prepared to fabricate the counter-electrode. Commercial Pt catalyst paste (Platisol T/SP, Solaronix, Switzerland) was deposited on the pre-drilled FTO by screen printing. The platinized counter-electrode was completed by sintering at 450 °C for 10 min. The prepared photo- and counter-electrode was assembled using thermoplastic hot-melt sealing sheets (SX 1170–60, Solaronix, Switzerland), 60 μm in thickness. A redox electrolyte consisting of 0.5 M LiI, 0.05 M I_2 and 0.5 M 4-tertbutylpyridine in acetonitrile was injected through the two pin holes on the counter-electrode. The DSC was completed by soldering to make the connection to the external circuit. The DSC used for the comparison with the simulation results was also fabricated using the same process.

The photovoltaic performance of the fabricated cells was measured under 1 sun (air mass 1.5, 100 mW/cm^2) using a source meter (Model 2400, Keithley Instrument Inc., USA). During the measurements, the cells were covered with a black mask except for the active area. The measured V_{OC} and J_{SC} of the representative cells were used to extract the voltage and current coefficient. The measured *I–V* data of the standard cell were used as the standard *I–V* characteristics. In addition, the fill factor (FF) and conversion efficiency (η) were calculated as the *I–V* characteristics of each sample. The simulation was conducted by using the PSIM software, which is a widely used commercial power electronic simulation program developed by the Powersim Inc.

3. Simulation and experimental results

3.1. Simulation theory

Fig. 1 shows the basic concept for obtaining the simulated *I–V* characteristics of the DSC in this study. The voltage coefficient (α_T) and current coefficient (β_T) are extracted from the representative experimental V_{OC} and J_{SC} data according to the different variables. In this study, the variable is the TiO_2 thickness. The thickness of the electrolyte layer is also changed along with the TiO_2 thickness variation because the thickness of the spacer is fixed as 60 μm. However, this can be ignored because the change of the electrolyte thickness below 120 μm does not have influence on the performance of DSC [10]. Therefore, it is assumed that the voltage and current coefficients mainly depend on the TiO_2 thickness in this simulation. Finally, the simulated *I–V* data are obtained by multiplying the coefficients according to the TiO_2 thickness and standard *I–V* data.

The detailed simulation algorithm is shown in the flow chart like the Fig. 2. As shown in the Fig. 2, the values of lower and higher range were selected based on the representative experimental data when the specific TiO_2 thickness (T) was inputted to simulate. And then, the coefficients were extracted using the inputted TiO_2 thickness and the selected values of the lower and higher range by the following formulae:

$$V_{TN} \equiv V_{TL} - \frac{T - T_L}{T_H - T_L}(V_{TL} - V_{TH}) \tag{1}$$

$$J_{TN} \equiv J_{TL} - \frac{T - T_L}{T_H - T_L}(J_{TL} - J_{TH}) \tag{2}$$

$$\alpha_T \equiv V_{TN}/V_{ST-OC}, \text{ and } \beta_T \equiv J_{TN}/J_{ST-SC} \tag{3}$$

where V_{TL}, J_{TL} and T_L are the open-circuit voltage, current density and thickness of the lower range according to the selected thickness, respectively; V_{TH}, J_{TH} and T_H are the open-circuit voltage, current density and thickness of the higher range, respectively, according to the inputted TiO_2 thickness; and $V_{ST\text{-}OC}$ and $J_{ST\text{-}SC}$ are the open-circuit voltage and current density of the standard cell, respectively. After extracting the coefficients, the voltage (V_{STC}) and current density (J_{STC}) of the standard cell were referred. Continuously, the simulated voltage (V_{NEW}) and current density (J_{NEW}) of the DSCs with the inputted TiO_2 thickness were generated using the following equation:

$$V_{NEW} = \alpha_T \cdot V_{STC}, \text{ and } J_{NEW} = \beta_T \cdot J_{STC} \tag{4}$$

A simulated *I–V* curve was plotted based on this data.

The simulation algorithm as above was coded using Microsoft Visual C++ based on the C-programming language. In the PSIM

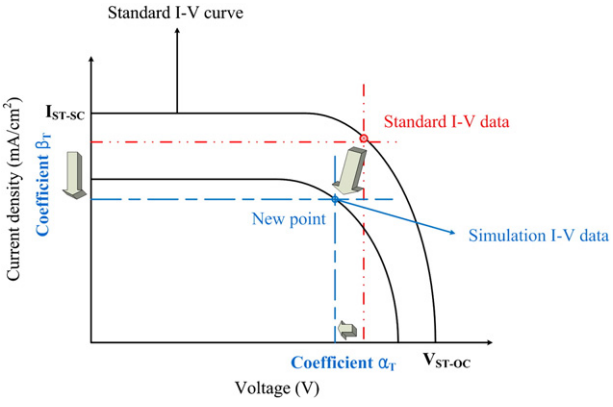

Fig. 1. Basic concept for the simulation of the DSC in this work.