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Enhanced electrical model for dye-sensitized solar cell characterization

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Abstract

The dye-sensitized solar cells (DSSC) have aroused in recent decades a growing interest from researchers in photovoltaic area, and those for their low cost and their performance very respectable (~11.2%). The physical and chemical phenomena that take place inside DSSC cells are complex compared to the conventional one. They are related to disordered and tangled nature of materials that made the recipe of these DSSC, such as TiO_2, electrolyte, and dye. In the present paper, we deliver a detailed theoretical model based on electrical considerations to study the impact of physical parameter of DSSC cell on the *J–V* characteristic, performance and photovoltaic efficiency. The DSSC cell is modeled as a "pseudo-homogeneous effective medium" consisting of a TiO_2 semi-conductor, dye absorber of light and electrolyte in order to study the transport and electrochemical phenomena. The model is resolved numerically using the Broyden–Fletcher–Goldfarb–Shanno (BFGS) approach and allow access to several physical parameters and their impact on the performance of the cell. The main target is to control theses parameters to get an optimized DSSC cell for a performing photovoltaic device.

Keywords: Dye-sensitized solar cell (DSSC); TiO_2; Electrical model; Parameters impact; *J–V* characteristics

1. Introduction

Dye-sensitized solar cells (DSSC) are thin film solar cells based on semiconductor grown between a photo-sensitized anode, photo-electrochemical material and an electrolyte (Nazeeruddin et al., 1993, 2001). They are called also Grätzel cell due to the name of their co-inventor (with O'Regan) O'Regan and Grätzel (1991). They became attractive due to their low cost and simple to make compared to other solar cell devices although their conversion efficiency is less than the best thin-film cells (Han et al., 2004). Most recently, due to their competitive price/performance ratio, DSSC have gained an important place among solar technologies. Their efficiency is more than 11.2% (Nazeeruddin et al., 1993, 2001; O'Regan and Grätzel, 1991; Han et al., 2004) with costs of production significantly lower compared to the conventional solar cells. However, not only technological problems (long-term stability) must be solved, but also physics of devices of this type of cells is not yet augur well in detail.

It is important to optimize the performance of DSSC and joint (theoretical and experimental) efforts were made and continue to progress nowadays. In theoretical side, quantitative modeling of the photovoltaic response of the DSSC is an important topic for improving the operation

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mechanisms and predicting new device performance (Peter, 2007; Topič et al., 2010; Bisquert and Mora-Seró, 2010). One of the most robust models that were developed recently, an analytical electrical model has emerged to explore different mechanisms responsible on DSSC's mode of operation. In fact, this classical model is based on diagram conduction phenomena by the introduction of macroscopic parameters. It studies the variations of these parameters in order to obtain an overview of optimized parameters for the development of manufacturing techniques. However, modeling a cell by an electrical circuit remains a challenging task as we need to connect the parameters of the model to the microscopic phenomena. It is therefore necessary to establish a robust model that allows us to know the internal properties of the cell (Halme et al., 2010; Onodera et al., 2010; Andrade et al., 2011; Wenger et al., 2011; Gentilini et al., 2012). The main goal of this model was also to see the impact of physical parameters on the operation mode of DSSC cells (Gentilini et al., 2012; Nithyanandam and Pitchumani, 2012; Joshi et al., 2013; Mitroi and Fara, 2013). These physical parameters are the thickness and morphology of TiO_2 layer, the mobility of electron and recombination rate (electron lifetime), spectrum of absorption of the dye, materials quality making the transparent conductive oxide (TCO) layers and their thickness effect. The main target of the numerical simulations is to extract information about the open circuit voltage V_{oc}, the short-circuit current density J_{sc}, the fill factor (FF), and then deduce the power conversion efficiency η were deduced and analyzed to judge on the quality of DSSC cell. All these issues are showing the need to look for an appropriate modeling for more control, development and optimization of DSSC cells performance.

In the present work, an electrical model of the dye-sensitized solar cell (DSSC) is introduced. The present model is well known as it follows the description of transport and the electrochemical phenomena that was presented previously by Ferber et al. (1998). This model takes into account the properties of electrons in the semiconductor and electrolyte (Ferber et al., 1998). Furthermore, the performance parameters of the cell are related directly to the material parameters. Our main contribution was to introduce the Broyden–Fletcher–Goldfarb–Shanno (BFGS) method in order to improve the model and investigate the influence of other parameters on the performance of the cell, such as: transient time, porosity of TiO_2, diameter and thickness of TiO_2, effective diffusion, and electron lifetime. The present model aims to be robust and complete to perform prediction of new DSS cells and their performance in the future.

2. Mathematical model of DSSC

The structure of a DSSC contains two conducting electrodes and an electrolyte, a redox couple I^-/I_3^- as shown in Fig. 1. The electrodes are constructed on glass substrates and coated with a transparent conducting oxide (TCO) layer (Perera et al., 2014). The working electrode consists of titanium dioxide (TiO_2) that is sensitized with a dye. The counter electrode is made with a catalyst material such as Pt, in order to promote the reduction of the oxidized form of the redox couple in the electrolyte. Indeed, the two conducting glass substrates were connected via the external circuit.

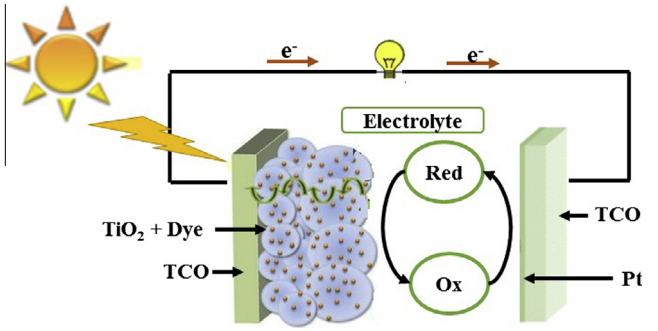

Fig. 1. Schematic diagram of the DSSC structure showing two conducting electrodes, an electrolyte and a redox couple I^-/I_3^-. The interconnected TiO_2 particles (blue gray) are covered with light-absorbing dye molecules (small brown dots). The free volume between two electrodes is filled with the electrolyte. TCO/TiO_2 interface or the electrolyte/platinum interfaces are colored in green (light and dark) color. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

We assume a simplified structure for the porous semi-conductor which is similar to that adopted by Ferber et al. (1998). The cell was modeled as an effective pseudo-homogeneous medium of thickness t_{TiO_2}. The pseudo- homogeneous medium consists of a nano-porous semi-conductor TiO_2, a dye and redox electrolyte, which are intermingled. Electro-actives particles (electrons e^- injected into the nano-porous TiO_2 layer after absorption of light by the dye, the reduction and oxidation of the redox electrolyte, and the positively charged cation cat^+) are involved in the process of moving according to different effective transport coefficients (Ferber et al., 1998). The continuity and transport equations are applied to all mobile charge carriers.

2.1. Chemical and electrochemical reactions

The dye (S) is grafted on the surface of a semi-conductor oxide in the form of a monolayer molecular (Fig. 2) (Andrade et al., 2011). It absorbs the solar rays that promote in a state electronically excited S^*, where it is able to inject an electron in the TiO_2 conduction band. Thus, the injected electrons pass through the layer then they are collected by a current collector, which allows directing them to an external circuit where their passage produces electrical energy. The return of the electron in the conduction band on the oxidized dye S^+ is much slower than the reduction of S^+ by the mediator in solution. The oxidized