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The effect of porosity on the current electron density at dye solar cell

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ABSTRACT

In this paper, we investigate the effect of the porosity on the current electron density (j_e) in a modeled dye solar cell (DSC). We have used electrical model for numerical simulation of the continuity, Poisson and transparent differential equations. The results show that by decreasing the porosity, the electron current density is increased which cause to improve cell efficiency. On the other hand by increasing the porosity the tri-iodide concentration ($n_{I_3^-}$) is decreased and iodide concentration (n_{I^-}) within DSC is increased which cause to increase j_e and improve the performance of the cell.

1. Introduction

It is expected that fossil fuels have a threat for the global economy in the coming years. Also because harmful ecological impact of conventional energy sources, it is obvious that development of clean alternative energy sources with easily and cheap accessible is a necessity. Since the solar energy is our only external energy source, which its energy is harness, clean, non-hazardous and infinite, satisfies the main objectives of all alternative energy strategies [1,2]. Solar cells convert sunlight to electricity. There are two ways for the development of solar cells. The first is to make them more cheaply at the low efficiency. The second is to make at a very high efficiencies and accepting higher costs [3]. Kinds of solar cells are silicon solar cells [4], thin film solar cells [5–7] and dye-sensitized solar cells (DSSCs) [8]. O'Regan and Grätzel announced dye-sensitized solar cell (DSSC) in 1991. Since then it has been continuously studied in various aspects because its low cost, noncomplicated technology, high efficiency and compared with conventional inorganic solar cells [1,9,10]. DSSCs generally consist of an active electrode (nanocrystalline titanium dioxide (TiO_2) deposited on the transparent conductive oxide (TCO) and dye adsorbed on it), an electrolyte (iodide/tri-iodide (I^-/I_3^-) redox couple), and a counter electrode comprising catalytic platinum film [1,9–11]. In order to investigate the complexity of the DSCs, simulation techniques are utilized [12,13]. Physical models provide powerful tools in optimizing DSCs. They link material parameters of the DSC with the electrical performance of the cell [14–16,10]. Charge transport in TiO_2 semiconductor film is important for the cell performance. Porosity effects on the charge transport and it act as a large surface area support for dye molecules.

In this paper, we evaluate effect of the porosity on the cell parameters within modeled DSC such as electron current density and distribution of the electron particle density, iodide and tri-iodide concentrations.

2. Physical model

DSCs are composed of several layers; including active electrode and counter electrode that the gap between them fill with electrolyte. The contact between the electrolyte and the platinized TCO at counter electrode is modeled as a redox electrode via the Nernst equation. The TiO_2/TCO

Contact (active electrode) is modeled as an ohmic metal-semiconductor contact. Equations are used within the TiO_2 and within the electrolyte. Electrons in the TiO_2 conduction band and the iodide, the tri-iodide, and the cations in the electrolyte are mobile charge carriers. We consider the transport of charge carriers which can be described by effective diffusion coefficient D or mobility μ [15]. Basic our model framework follows from work by Ferber et al. [16]. Dye molecule absorbs light and excite, the excited state electrons inject into TiO_2 conduction band and dye is regenerated again. These processes are fast reactions [10]. We can assume that absorption of a photon is simultaneous with electron injection and dye regeneration follow from chemical reaction [16,17] as follow:

$$3I^- \rightarrow I_3^- + 2e^- \quad (1)$$

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The continuity equation governing on the charged particles (iodide, tri-iodide, cations in electrolyte and electrons in conduction band TiO_2) can be written as:

$$\frac{1}{e_0}\frac{dj_e}{dx} = k_e n_e \sqrt{\frac{n_{I_3^-}}{n_{I^-}}} - \int \alpha\phi(\lambda)e^{-\alpha(\lambda)x}d\lambda \quad (2)$$

α is absorption coefficient which is depended on the porosity. When $p \geq 0.41$, the relation between α and p is described by Eq. (3) [18]:

$$\alpha = 2568(1-p)(p+2.89) \quad (3)$$

$\phi(\lambda)$ is spectral incident photon flux density and λ is wavelength [19–22]:

$$\frac{1}{e_0}\frac{dj_{I^-}}{dx} = -\frac{3}{2e_0}\frac{dj_e}{dx} \quad (4)$$

$$\frac{1}{e_0}\frac{dj_{I_3^-}}{dx} = \frac{1}{2e_0}\frac{dj_e}{dx} \quad (5)$$

$$\frac{1}{e_0}\frac{dj_c}{dx} = 0 \quad (6)$$

The electric field could be obtained by Poisson's equation [23]:

$$\frac{dE}{dx} = \frac{e_0}{\varepsilon\varepsilon_0}[n_c(x) - n_e(x) - n_{I^-}(x) - n_{I_3^-}(x)] \quad (7)$$

Charge carrier could be described by using transport equations (Eqs. (9)–(12)). In these equations D is diffusion coefficient. When $p \geq 0.41$, the relationship of D and p describe as Eq. (8) [18]:

$$D = 4 \times 10^{-4}(0.76 - p)^{0.82} \quad (8)$$

$$\frac{1}{e_0}j_e = D\frac{dn_e}{dx} + \mu_e n_e E \quad (9)$$

$$\frac{1}{e_0}j_{I^-} = D\frac{dn_{I^-}}{dx} + \mu_{I^-} n_{I^-} E \quad (10)$$

$$\frac{1}{e_0}j_{I_3^-} = D\frac{dn_{I_3^-}}{dx} + \mu_{I_3^-} n_{I_3^-} E \quad (11)$$

$$\frac{1}{e_0}j_c = -D\frac{dn_c}{dx} + \mu_c n_c E \quad (12)$$

μ is the mobility of charge carriers. Relation between D and μ is described by Einstein relation [16]:

$$D = \frac{KT}{e_0}\mu \quad (13)$$

The boundary integrals over the cell to be described as Eqs. (14)–(16). Total number of the cations within the cell is constant.

$$\int n_c dx = \int n_c^0 dx = n_c^0 \cdot d \quad (14)$$

Also total number of iodine ions in the cell is equal to its initial concentration:

$$\int \left(n_{I_3^-} + \frac{1}{3}n_{I^-}\right)dx = \left(n_{I_3^-}^0 + \frac{1}{3}n_{I^-}^0\right)\cdot d \quad (15)$$

For every three iodide ions, we have two conduction band electrons

$$\int \left(\frac{1}{2}n_e + \frac{1}{3}n_{I^-}\right)dx = \left(\frac{1}{2}n_e^0 + \frac{1}{3}n_{I^-}\right)\cdot d \quad (16)$$

In addition the total amount of negative charges within the cell equal to the total of positive charges [16,24,25].

Final boundary condition in the cell is defined as internal voltage of DSSCs:

$$U_{int} = \frac{1}{e_0}[E_F^n(0) - E_{Redox}] \quad (17)$$

The quasi-Fermi level E_F^n depends on the electron density

$$E_F^n(0) = E_{CB} + KT\ \ln\frac{n_e(0)}{N_{CB}} \quad (18)$$

E_{CB} is the energy of the conduction band edge, N_{CB} the effective density of states in the TiO_2 conduction band, K is Boltzmann constant and T is absolute temperature in Kelvin.

$$N_{CB} = 2\left(\frac{2\pi m_e^* KT}{h^2}\right)^{\frac{3}{2}} \quad (19)$$

The redox energy E_{Redox} of the platinum electrode may be written as the sum of its redox energy E_{Redox}^{OC} (open-circuit condition), and the deviation from the equilibrium in operation point, which is named overvoltage U_{pt} [16,22]:

$$E_{Redox} = E_{Redox}^{OC} + e_0 U_{pt} \quad (20)$$

3. Result and discussion

Described model in Section 2 together with boundary condition is solved. There are six coupled first-order ordinary differential equations. The integral boundaries are converted to differential equations and added to the six equations. We solved our model by using relaxation method with considering two point boundary problem ($x = 0$ and $x = d$). The important parameters used in simulation are shown in Table 1. Figs. 1–6 show the results of simulation. We derived the results with reasonable values and compared with several literature sources [16,22] for testing the credibility of the model and program.

Fig. 1 is shown the influence of porosity on the electron current density within the modeled DSC. We know that polyethylene

Table 1
Parameters used in the model.

Parameter	Symbol	Value
Electron charge	e_0	1.6×10^{-19}
Initial I^- concentration	$n_{I^-}^0$	2.71×10^{20} cm^{-3}
Initial I_3^- concentration	$n_{I_3^-}^0$	3.01×10^{19} cm^{-3}
Initial electron concentration	n_e^0	10×10 cm^{-3}
Effective electron mass	m_e^*	$5.6\, m_e$
Effective relative dielectric constant	ε	50
Difference of conduction band energy and redox energy of electrolyte	$E_{CB} - E_R$	0.93 eV
Incident spectral photon flux density	$\phi(\lambda)$	*AM*1.5

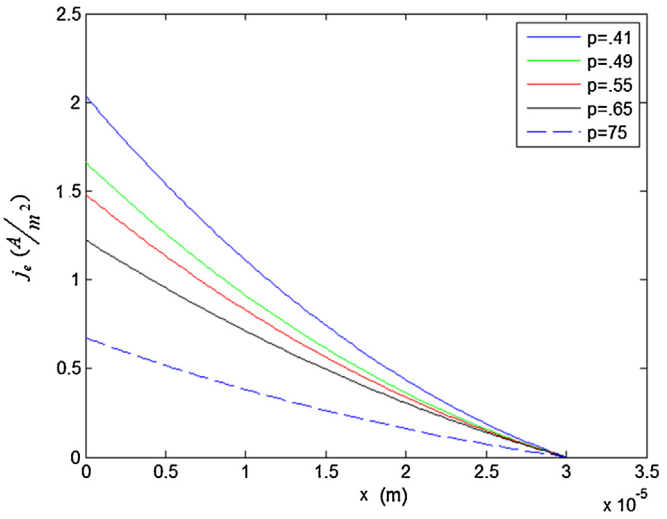

Fig. 1. The electron current density within the modeled DSC under different porosity.