Proceedings of the International Congress on Advances in Applied Physics and Materials Science, Antalya 2011

Design of Hybrid Solar Cell Based on Dye-Sensitized TiO_2 Nanoparticles with Conjugated Polymer

K. Abbasian*, A. Rostami and S. Pourkhorshidi

School of Engineering-Emerging Technologies, University of Tabriz, Tabriz 51666, Iran

In this paper, we have proposed dye-sensitized hybrid solar cell based on TiO_2 nanoparticles as a medium for electron transport and conjugated polymers as hole-conductor, where dye molecules absorb solar radiation and create electron–hole pairs. This solar cell can be a better alternative to conventional electrolyte based dye-sensitized solar cells, because of enhanced characteristics of performance. We have simulated it numerically, to study essential characteristics of the structure such as electron, hole and their current densities and internal electric field in two operating conditions of open-circuit and short-circuit cases. Then current–voltage characteristic diagram has been plotted and energy conversion efficiency calculated.

PACS: 82.35.Np, 88.40.hj

1. Introduction

In 2008, world's total energy consumption was about 15 TW and 80 to 90 percent of that was supplied from fossil fuels. It is predicted that up to 2030 the world's required total energy will be doubled due to world's population growth and economic growth. Also, fossil fuels price and impact on the environment, namely "green-house" effect, is an important issue. Then, there is a growing need for clean and reproducible energy sources. Solar energy is known as the main source.

Among several solar cell structures, an important one is dye-sensitized solar cell (DSSC). DSSC is composed of nanoporous TiO_2 layer sensitized with small dye molecules, deposited on a transparent conductive oxide (TCO) glass doped with fluorine as anode, and a TCO deposited by platinum as counter electrode; and penetrating redox electrolyte consistent of iodide and tri-iodide.

Because of some disadvantages of liquid electrolyte, namely corrosion and evaporation, and in order to conduct hole carriers, other materials such as conjugated polymers can replace the electrolyte. So, dye-sensitized hybrid solar cell (DSHSC) with TiO_2 nanoparticles and conjugated polymers is introduced. Ferber et al. [1] developed an electrical model for DSSC, but they assumed an electron transfer mechanism without any traps in TiO_2 film. Hybrid heterojunction solar cells based on nanocrystalline mesoporous TiO_2 and hole conducting material have been studied and the energy levels of the solid-state electrolyte have been established in [2].

As shown in Fig. 1, the DSHSC is composed of a transparent conductive oxide glass doped with fluorine, and a layer of metal oxides such as TiO_2 or ZnO, which exhibit semiconducting properties; and a layer of their nanoparticles. For holes conducting, conjugated polymer is used. Another TCO doped with Au or Ag is used to form the counter electrode [3].

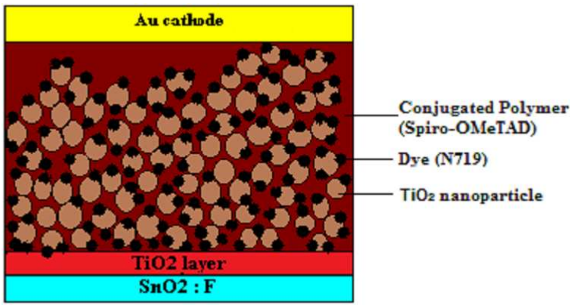

Fig. 1. Schematic of a DSHSC with TiO_2 nanoparticles, dyes and conjugated polymers.

The conjugated polymers often show metallic or semiconducting properties. Then, in hybrid solar cells conjugated polymers can act as solar radiation absorber and producer of free electrons, while in hybrid solar cells with TiO_2 nanoparticles and dyes, dye molecules mainly absorb solar radiation and conjugated polymers act as hole conducting material.

2. Theory and mathematical background

These cells are a kind of excitonic solar cells, because solar radiation causes the dye molecules to absorb a photon and one of its electrons goes from the highest occupied molecular orbital (HOMO) to lowest unoccupied

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[*] corresponding author; e-mail: `k_abbasian@tabrizu.ac.ir`

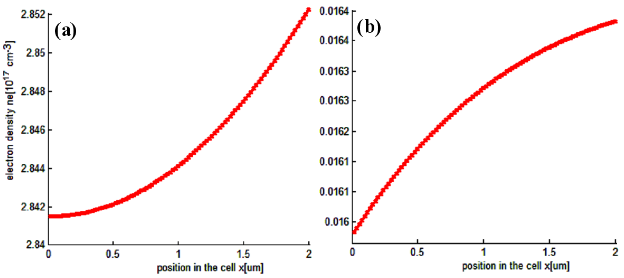

Fig. 2. Electron density (a) in open-circuit case, and (b) in short-circuit operating condition, similar and symmetrical with hole density.

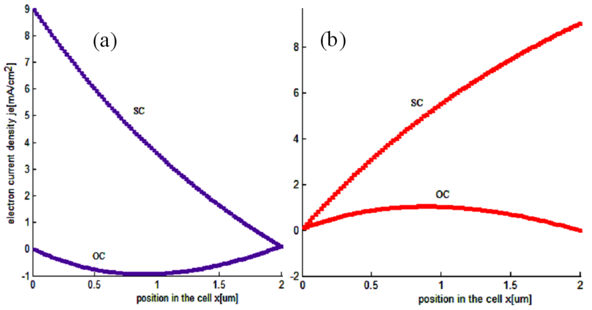

Fig. 3. Current densities of (a) electron and (b) hole; in short-circuit (SC) and open-circuit (OC) conditions.

molecular orbital (LUMO) or simply, the dye changes to the excited state which is denoted by D* as an exciton.

As electron transfer from dye LUMO to the $\mathrm{TiO_2}$ conduction band occurs, exciton dissociates and a hole is made in the dye molecule, so the dye needs an electron and if does not take it rapidly, decomposes and cell loses its operation, consequently electron transfers from the conduction band of the conjugated polymer to the conduction band of the dye molecules or equally the hole is transferred from the LUMO of the dye to the conjugated polymer.

In the next step induced electrons and holes transfer to the electrodes through $\mathrm{TiO_2}$ and conjugated polymer. Then, we will encounter two carrier transport mechanisms: (a) transfer of the electron in the interconnected network, (b) the hole transfer through the conjugated polymer to the cathode.

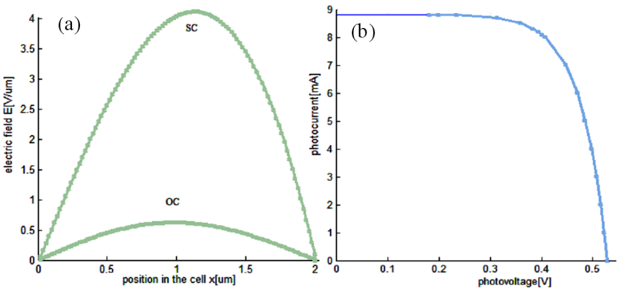

Fig. 4. (a) Internal electric field distribution, (b) I–V curve of the SC.

Electrons and holes current densities follow from the continuity equation, and the electric field is obtained from the Poisson equation. After some mathematical manipulations all of the cell equations can be summarized as

$$-\frac{1}{e_0}\frac{\mathrm{d}j_{\mathrm{e}}(x)}{\mathrm{d}x} = \alpha I_0 \exp(-\alpha x) - k_{\mathrm{e}}[n_{\mathrm{e}}(x) - n_0]\,, \tag{1}$$

$$\frac{1}{e_0} j_{\mathrm{e}}(x) = D_{\mathrm{e}}\frac{\mathrm{d}n_{\mathrm{e}}(x)}{\mathrm{d}x} + \mu_{\mathrm{e}} n_{\mathrm{e}}(x)E(x)\,, \tag{2}$$

$$\frac{1}{e_0}\frac{\mathrm{d}j_{\mathrm{h}}(x)}{\mathrm{d}x} = \alpha I_0 \exp(-\alpha x) - k_{\mathrm{h}}[n_{\mathrm{h}}(x) - n_{\mathrm{h}_0}]\,, \tag{3}$$

$$\frac{1}{e_0} j_{\mathrm{h}}(x) = -D_{\mathrm{h}}\frac{\mathrm{d}n_{\mathrm{h}}(x)}{\mathrm{d}x} + \mu_{\mathrm{h}} n_{\mathrm{h}}(x)E(x)\,, \tag{4}$$

$$\frac{\mathrm{d}E(x)}{\mathrm{d}x} = \frac{e_0}{\varepsilon\varepsilon_0}[n_{\mathrm{h}}(x) - n_{\mathrm{e}}(x)]\,, \tag{5}$$

where α denotes dye absorption spectrum, I_0 is the incident photon flux density. D_{e}, μ_{e} and e_0 are diffusion coefficient, mobility, and elementary charge of the electron, respectively. $E(x)$ is the internal electric field that is induced because of the charge imbalance. k_{e} and k_{h} are the back reaction rates, $n_{\mathrm{h}}(x)$, D_{h} and μ_{h} are density, diffusion coefficient and mobility of the hole, respectively.

Using parameters of Table, we can solve the coupled set, using the following boundary conditions:

$$E(x=0) = E(x=d) = 0\,, \quad j_{\mathrm{e}}(x=d) = 0\,,$$

$$j_{\mathrm{h}}(x=0) = 0\,, \quad \int_0^d [n_{\mathrm{h}}(x) - n_{\mathrm{e}}(x)]\,\mathrm{d}x = cte\,. \tag{6}$$

3. Simulation results

In this section, a 2 μm thick DSHSC under open circuit and short circuit operating conditions has been simulated. Obtained simulation results for carriers densities have been shown in Fig. 2, current densities have been demonstrated in Fig. 3, then internal electric field distribution and I–V curve of the solar cell have been demonstrated in Fig. 4.

4. Conclusion

A hybrid dye-sensitized solar cell with about 2 μm thickness is modeled and the I–V diagram is plotted which results in efficiency of 3.24%, which is low compared to the 11% efficiency calculated for DSSC. However, because of known advantages of this structure to the conventional DSSC, some trials have to be done to improve its efficiency.

TABLE

Used parameters in the DSHSC simulation [2–4].

Parameter	Sign	Numerical value
diffusion coefficient of electrons in conduction band of TiO_2	D_0	$0.05\ cm^2/s$
electron lifetime in the TiO_2 conduction band	τ_0	$10^{-3}\ s^{-1}$
TiO_2 conduction band electrons density of states	$S_t(0)$	$10^{17}\ m^{-3}\ (eV)^{-1}$
asymmetry parameter	β	0.62
trap density in conduction band of TiO_2	N_c	$10^{20}\ cm^{-3}$
trap density in the conjugated polymer	N_0	$2.9 \times 10^{19}\ cm^{-3}$
relative dielectric constant of the mixed medium	ε_0	3
distribution width of the density of states of conjugated polymer	σ_1	65 meV
absolute temperature	T	300 K

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