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INVESTIGATION OF THE EFFECT OF POLYMERIC AND NON-POLYMERIC MATERIALS IN THE HOLE TRANSFER LAYER ON THE PERFORMANCE OF PEROVSKITE SOLAR CELL

DELİK TRANSFER TABAKASINDAKİ POLİMERİK VE POLİMERİK OLMAYAN MALZEMELERİN PEROVSKİT GÜNEŞ HÜCRELERİ PERFORMANSINA ETKİSİNİN ARAŞTIRILMASI

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ABSTRACT

In recent decades, due to advances in various industries, the use of renewable energy sources has increased significantly. Solar cells are one of the important tools in the use of renewable energies. Between the different types of solar cells, recently, perovskite solar cells, because of some advantages like low costs of materials used in their fabrication, simple manufacturing process, and high conversion efficiency, have gained the attention of many researchers. Emerging technology and recent research activities have helped perovskite solar cells to achieve high efficiency, which is highly dependent on the components and structures of the solar cell system. One way to achieve high efficiency is to use polymeric and non-polymeric materials as electron transporters (ETMs), hole transporters (HTMs), or as a stimulus to increase the performance durability of perovskite solar cells. Simulation tool is a very effective tool for designing solar cells. In this study, by using COMSOL Multiphysics software, the effect of using different hole transfer layers, both polymeric and non-polymeric, has been investigated. For this purpose, three HTM layers (Spiro-OMETAD, CuSCN, P3HT) have been investigated. The results represented that the efficiencies for these three materials were 16.8%, 15.7%, 12.1%, respectively, and Spiro-OMETAD has been more efficient.

Keywords: COMSOL, solar cells, perovskite, polymers, efficiency.

ÖZET

Son yıllarda, çeşitli endüstri ve teknolojilerdeki gelişmeler nedeniyle yenilenebilir enerji kaynaklarının kullanımı önemli ölçüde artmıştır. Güneş hücreleri, yenilenebilir enerjilerin kullanımında en önemli araçlardan biridir. Farklı güneş hücreleri türleri arasında, son zamanlarda perovskit güneş hücreleri, imalatlarında kullanılan malzemelerin düşük maliyeti, basit üretim süreci ve yüksek dönüşüm verimliliği (aynı fiyat aralığındaki diğer güneş hücrelerine kıyasla) gibi bazı avantajlara sahiptir. Gelişen teknoloji ve son araştırma faaliyetleri, güneş hücreleri sisteminin bileşenlerine ve yapılarına büyük ölçüde bağlı olduğunu göstermiştir. Bu sebeple perovskit güneş hücreleri, yüksek verimliliğe ulaşmak için birçok araştırmacının dikkatini çekmiştir. Yüksek verim elde etmenin bir yolu, polimerik ve polimerik olmayan malzemeleri elektron taşıyıcılar (ETM'ler), delik taşıyıcılar (HTM'ler) veya perovskite güneş

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hücreleri performansını, kararlılığını ve dayanıklılığını artırmak için bir uyarıcı olarak kullanmaktır. Güneş hücreleri simülasyonu ve modellemesi, güneş hücreleri tasarlamak ve üretmek için önemli ve çok etkili bir araçtır. Bu çalışmada, COMSOL Multifizik yazılımında bir simülasyon aracı kullanılarak, hem polimerik hem de polimerik olmayan farklı delik transfer katmanlarının kullanılmasının etkisi araştırılmıştır. Bu amaçla üç HTM katmanı (Spiro-OMETAD, CuSCN, P3HT) incelenmiştir. Sonuçlar, bu üç malzemenin verimlilikleri sırasıyla 16.8%, 15.7%, 12% olarak bulundu ve Spiro-OMETAD'ın daha verimli olduğu belirlendi.

Anahtar Kelimeler: COMSOL, güneş hücreleri, perovskit, polimerler, verimlilik.

INTRODUCTION

The way to obtain electrical energy from the sun is to take advantage of the photovoltaic phenomenon. Given that the sun is a good source of energy in terms of cleanliness, availability, and absence of carbon dioxide, so it can play the most important role in providing human energy sources in the future (Salihmuhsin & Aldwihi, 2019). According to research, the amount of solar radiation on the earth's surface in one hour is more than the total energy used by the world's population in one year. With these interpretations using the energy obtained from the sun to solve problems due to lack of energy resources is a good option that occurs via solar cells. Solar cells are semiconductor materials that convert sunlight directly onto their surfaces into electrical energy (Ozcalık, Yılmaz, & Kılıc, 2013). Among all types of solar cells, perovskite solar cells have been further studied for reasons such as low device fabrication cost, good performance, and high efficiency.

In 2009, Miyasaka et al. first used a thin layer of perovskite on top of the mesoporous titanium oxide layer as a visible light sensitizer. The efficiency (PCE) for the reported cell was about 4% (Kojima, Teshima, Shirai, & Miyasaka, 2009). Studies in this area have continued in recent years and its performance has increased to about 22%. The Perovskite solar cell has become an interesting global issue due to its rapid development and high efficiency, as well as its easy and low-cost fabrication methods. The raw materials and methods of construction of this type of cells are very diverse and extensive, therefore, using them is a good option. The structure of a perovskite-based solar cell contains an FTO-coated glass, a layer of TiO_2 as the electron transporter (ETM), a perovskite light-absorbing layer, a hole-transfer layer (HTM), and a back electrode. The performance of this type of cell is that the perovskite layer acts as a light-absorbing layer that, like any other semiconductor material, absorbs some of the incoming photons of sunlight. With the absorption of each photon, a pair of electrons and a hole are created. The electrons and holes produced are scattered on either side of the perovskite layer; electrons to the ETM and holes to the HTM. Each of these layers has advantages and disadvantages, which by changing each of them, the efficiency and performance of the cell can be affected. Zandi et al. in 2019 compared two simple and tandem $CH_3NH_3PbI_3$ based perovskite solar cells without and with an additional second $CH_3NH_3SnI_3$ absorber layer, respectively. Results represented that adding $CH_3NH_3SnI_3$ helps to efficiency improvement about 1% and efficiency increased from about 14% to 15% (Zandi & Razaghi, 2019). Also in 2016, Tan et al. investigated the influence of using different transmitting layers on the main parameters of the solar cell in which the $MAPbI_3$ layer was used. The results showed that the values of the main parameters for Spiro-OMETAD were better than the rest of the material (Tan et al., 2016).

In this work, given the importance of the material used in the hole transfer layer and the effect it has on the efficiency of the perovskite solar cell, our goal is to obtain the current-voltage characteristic (J-V) and finally to evaluate the efficiency of the solar cell through simulation study. The software package utilized in the present study is COMSOL-Multiphysics software. Here the purpose is to examine using different materials effects in the HTM layer on the efficiency. Therefore, to investigate this effect, we used Spiro-OMETAD, CuSCN, and P3HT materials as hole transporting layers.

MATERIALS AND METHODS

The perovskite solar cell structure utilized in this study with layers that are of a certain thickness is shown in Fig.1. In this figure, the Au is considered as a cathode, Spiro–OMETAD as the HTM, the perovskite layer ($CH_3NH_3PbI_3$) as an absorber layer, TiO_2 as the ETM, FTO as an anode, and finally the air. In order to simulate the aforementioned perovskite solar cell structure, in the present work, the COMSOL-Multiphysics software was utilized. There are some reasons for the selection of this simulation tool in this work. One of the advantages of COMSOL-Multiphysics software that has caused the proper selection of this software as a modeling environment is in employing FEM solution method, that develops the ability to model complex structures (which have unusual boundary conditions). Two type of optical and electrical physics were employed in the software for the purpose of this study's simulation.

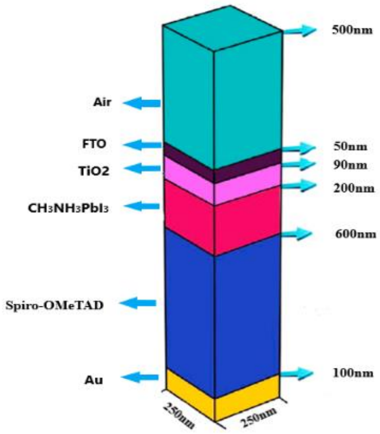

Figure 1. The Considered Perovskite Solar Cell Schematic of The Geometry.

Optical Part

In the optic section by using the Wave optic module, we finally want to obtain the photogeneration rate. The equations used in this part are as follows:

$$\nabla \times (\nabla \times E) - K_0^2\, \varepsilon_r E = 0 \tag{1}$$

$$K_0 = \frac{2\pi}{\lambda}$$

$$\varepsilon_r = (n - ik)^2$$

The K_0 is the wave-vector and ε_r is relative permittivity, both functions of the wavelength (λ).

By solving Eq. (1), the electric field intensity is obtained in the whole structure. It is then calculated using the intensity of the electric field, from the relation between the photogeneration rate per wavelength in the whole structure (Deceglie, Ferry, Alivisatos, & Atwater, 2012).

$$G_{photo}(\lambda) = \frac{\varepsilon''|E|}{2h} \tag{2}$$

In this equation, h is the Plank constant, and ε" is the imaginary part of the ε_r.

In this study, the initial sun-light power is 1000 W/m^2. The AM 1.5G spectrum is also used as input power for wavelengths between (300-1000 nm). There is also another relation for determining the total generation rate (G_{tot}):

$$G_{tot} = \int_{\lambda_{min}=300[nm]}^{\lambda_{max}=1000[nm]} G_{photo}(\lambda)\, d\lambda \tag{3}$$

Electrical Part

For the electrical part, the semiconductor module is utilized to determine the density of the carriers and, finally, to achieve the current voltage (J-V) of the solar cell. In this part, the Poisson's equation and the electrons and holes continuity equations are solved simultaneously.

$$\nabla \cdot (\varepsilon_s \nabla \emptyset) = -\rho \tag{4}$$

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla j_n + G_n - U_n \tag{5}$$

$$\frac{\partial p}{\partial t} = \frac{1}{q}\nabla j_p + G_p - U_p \tag{6}$$

In the above equations, ε is the electric potential, q is the electron charge, ε_s is the semiconductor permeability constant, G_n and G_p are the total generation rates of electron and hole, U_n and U_p refers to the rates of electrons and holes recombination, respectively. ρ is the charge density obtained from the following equation:

$$\rho = (p - n + N_A - N_D) \tag{7}$$

In this equation (eq. 7), n and p are the concentration of electron and hole, N_A and N_D refer to density of electron acceptor and donor, respectively. J_n and J_p in relationships are defined as the density of electrons and holes, respectively.

$$J_n = -q\mu_n n\nabla\emptyset + qD_n\nabla n \tag{8}$$

$$J_p = -q\mu_p p\nabla\emptyset + qD_p\nabla p \tag{9}$$

The required parameters for each layer are given in Table 1. These parameters were taken from the materials library or manually from the relevant literature (Zhou et al., 2016) and (Karimi & Ghorashi, 2017). The simulation was done at 300 K.

Table 1. Different Properties of Cell Layers in This Study. (Kojima et al., 2009; Dronov, Shevyakov, Belov, & Poltoratskii, 2009; Jaffe et al., 2010; Pattanasattayavong et al., 2013; Gavrilov,; Minemoto & Murata, 2014; Zhou et al., 2016; Zhang, Chen, & Yan, 2016)

Parameter	TiO_2	$CH_3NH_3PbI_3$	Spiro-OMETAD	CuSCN	P_3HT
Thickness[nm]	90	200	600	600	600
ε_r	9	6.5	3	10	3
E_g (eV)	3.2	1.55	3	3.4	1.05
χ (eV)	4	3.93	2.45	1.9	3.9
μ_n/ μ_p (cm^{-2}/VS)	20/10	50/50	2/0.01	1×10^{-4}/0.01	10^{-4}/10^{-4}
N_c (cm^{-3})	1×10^{19}	1.66×10^{19}	1×10^{20}	1.79×10^{19}	1×10^{20}
N_v (cm^{-3})	1×10^{19}	5.41×10^{19}	1×10^{20}	2.51×10^{19}	1×10^{20}
N_A (cm^{-3})	-	5×10^{13}	5×10^{18}	5×10^{18}	1×10^{16}
N_D (cm^{-3})	5×10^{18}	-	-	-	-
τ_n/ τ_p [ns]	5/2	8/8	0.1/0.1	5/5	1.8/1.8

RESULTS AND DISCUSSION

By obtaining the total generation rate (Gtot) and defining it as a semiconductor module and determining the boundary conditions, the simulation was done and the voltage-current characteristic was calculated.

After applying the boundary conditions, the voltage-current characteristic is obtained. The results were indicated in Fig.2 in the comparable form. The area under the curve represents the final electrical power that was generated by the cell. It is obvious that the cell containing Spiro-OMeTAD as a small molecule type hole transport layer, considerably generates more electricity compared to others.

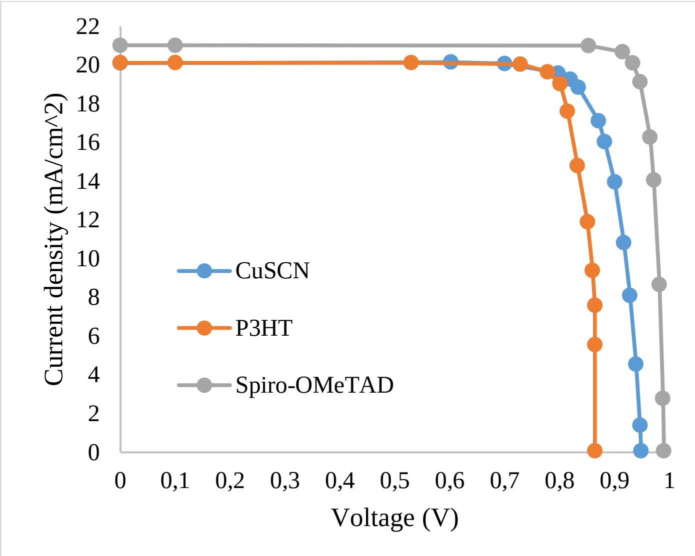

Figure 2. Current-Voltage (J-V) Curve of The Cell Using Different Mentioned HTMs

Photovoltaic parameters of a simulated perovskite solar cell were extracted from the Current-voltage (J-V) characteristics. According to the results obtained in Table 2, among the hole transfer layers, Spiro-OMETAD had the highest efficiency of 16.8% and the highest performance, followed by CuSCN and P3HT with returns of 15.7% and 12.1%, respectively. Besides, short-circuit current represented almost close for all HTM candidates. Moreover, results of open-circuit voltage confirmed that P3HT generates less voltage compared to the others (0.864 compared to 0.949 and 0.989). The fill factor of these materials showed almost the same amount for all of them. The aforementioned simulation results were compared and validated with experimental results (Zandi & Razaghi, 2019).

Table 2. The Photovoltaic Parameters Obtained for Different HTMs

structure	J_{SC} (mA/cm^2)	V_{oc} (v)	FF (%)	PCE (%)
Spiro-OMETAD based	21.02	0.989	0.82	16.8
CuSCN based	20.12	0.949	0.83	15.7
P_3HT based	20.12	0.864	0.84	12.1

CONCLUSION

Today, solar cells have become excellent sources of electricity generation due to their suitable and renewable properties. In recent years, newly developed perovskite solar cells have been considered by researchers because of their high efficiency and low cost. These types of solar cells are composed of different layers, the change of each of which can affect the efficiency and function of the cell. In this study, the effect of using different hole transfer layers (polymer-non-polymer) using COMSOL simulation software has been investigated. The hole transfer layers used in this work were: Spiro-OMETAD, CuSCN, P3HT. The results showed that the best efficiency belonged to small molecule and non-polymeric Spiro-OMETAD which was equal to 16.8%.

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