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بررسی سه بعدی اثرات تغییر دما و ماده انتقال دهنده حفره بر عملکرد سلول خورشیدی پروسکایت

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چکیده - اخیرا سلول‌های خورشیدی مبنی بر ارگانو متال هالید پروسکایت‌ها، پیشرفت‌های چشمگیری داشته‌اند. این ساختارها ویژگی‌هایی همچون چگالی نقص پایین، قابلیت تحرک بالای حامل‌ها و طیف جذبی گسترده، را دارا هستند. در این مقاله، تکنیک عددی سه بعدی تفاضل‌های محدود، برای شبیه سازی سلول‌های خورشیدی پروسکایت مسطح، استفاده شده است. مدل تلفیقی الکتریکی و نوری برای تشخیص پارامترهای کلیدی سلول خورشیدی شبیه‌سازی شده استفاده می‌شود. تأثیر تغییرات دما، و جایگزینی ماده‌ی CuSCN با ماده‌ی Cu_2O بر عمل‌کرد سلول-های خورشیدی بررسی شده است. تغییر ماده‌ی ذکر شده منجر به تغییر J_{sc} و FF شده است. با توجه به نتایج شبیه سازی‌ها، بهترین بازده ٪ ۱۴/۳۲ برای سلول خورشیدی حاصل می‌شود.

کلید واژه- سلول خورشیدی، پروسکایت، دما، شبیه سازی سه بعدی و HTM.

3D Investigation of Temperature and Hole Transport Material Variation on Performance of Perovskite Solar Cell

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Abstract- Recently, organo-metal halide perovskite solar cells based on planar architecture have demonstrated an exceptional progress These structures show lower defect density, high carrier mobility, and broader absorption spectra in compare to other solar cells. In this work a 3D finite element method (FEM) technique is used to simulate a planer perovskite solar cell. Coupled electrical-optical modeling is constructed to fully characterize the proposed device. We investigate variation of short circuit current (J_{sc}), open circuit voltage (V_{oc}) and fill factor (FF) in different temperature ranges (280-340 K). Also, the effect of material replacement (Cu_2O material instead of CuSCN), as hole transport material (HTM), has been investigated on solar cell performance. It is caused to change Jsc. Based on the result the best PCE is 14.32%. These simulation results open up a way to find accurate design parameters in solar cell with best performance.

Keywords: Solar cell, perovskite, temperature, 3D simulation and HTM

1 Introduction

Nowadays, Solid-state organo-metal halide perovskite solar cells (PSCs) have revolutionized solar cell industry. This new kind of solar cell such as MAPbX3 (MA= CH3NH3+; X = Cl^-, Br^-, I) has demonstrated an exceptional progress in solar cell power conversion efficiency (PCEs) from 3.81% for $MAPbI_3$ to over 20% [1, 2, 4]. high carrier mobility [3, 4], Long carrier diffusion length [3, 4], and long absorption coefficient [3, 4] are promising characteristics of perovskite materials..

Device simulation gives a better description of physical mechanism in solar cells. However, the number of reported simulations in this field are few. Therefore, in this work we present a three-dimensional (3D) PSC based on the finite-element method (FEM) from the "COMSOL Multiphysics" software package. Firstly**,** we validate our simulation results with previous experimental investigations [5]. Then, the effect of temperature variation and hole transport material (HTM) changes, are examined. It is shown that these variations, have an effective role on design of high PCE PSCs.

2 Theory and modelling

A schematic of the solar cell structure has been represented in Fig. 1. As it can be seen in this figure, a n-i-p solar cell with TiO_2 n-type layer as electron transport material (ETM) layer, $CH_3NH_3PbI_3$ as intrinsic layer and CuSCN p-type layer as HTM layer, is considered. Firstly, presented model is validated with previously published work [5]. Proposed n-i-p PSC structural parameters are taken as follow: a width of 250nm and a depth of 250 nm. Also, the structure includes five layers of: Air (500 nm thick), FTO (50 nm), TiO_2(90 nm), CH_3 NH_3 PbI_3(200 nm), CuSCN (600 nm,) and Au (100 nm), (see Fig. 1). Generally, our presented model consists of two parts of optical and electrical.

2.1 Optical Model

The Wave Optic module has been used in order to solve Maxwell's equations in the frequency domain. It is expressed as follow:

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

where, E is electric field, k_0 is wave-vector and ε_r is Complex Relative Permittivity $\varepsilon_r=(n-ik)^2$, which is a function of wavelength (λ).

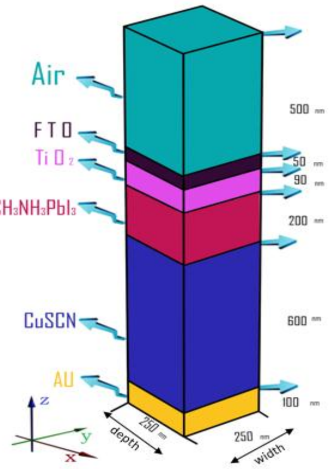

Figure 1: A schematic of perovskite solar cell (PSC).

With known amount of E, the photo-generation rate per each wavelength (G_{photo} (λ)), can be calculated as follow:

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

where h is the plank constant, ε'' is the imaginary part of the ε_r. For G_{photo} (λ) calculation, AM1.5G was used as the input power. The complex refractive indexes of FTO, CuSCN, TiO_2, $CH_3NH_3PbI_3$ and Au are taken from previously measured data [6-9]. Total generation rate (G_{tot}) is calculated by integration over the wavelength ranges. The results of these calculations have been presented in Fig. 2.

2.2 Electrical model

To evaluate current density-voltage (J-V) characteristics, semiconductor module from COMSOL software, is used. This module is based on solving Poisson and Continuity equations. It is expressed as below:

$$\nabla.(\varepsilon_s\nabla\phi)=-\rho \tag{3}$$

$$\frac{\partial n}{\partial t}=\frac{1}{q}\nabla j_n+G_n-U_n \tag{4}$$

$$\frac{\partial p}{\partial t}=\frac{1}{q}\nabla j_p+G_p-U_n \tag{5}$$

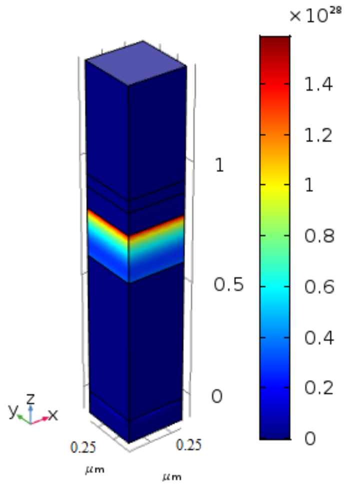

Figure 2: G_{tot} in PSC

where ϕ is electrostatic potential. q is electron charge. ε_s is semiconductor permittivity, G_n and G_p are total generation rates, U_n and U_p are recombination rates of electron and holes respectively. ρ is a charge density, J_n and J_p are current density of electron and hole. Calculated amount of G_{tot} in wave optic module, is replaced with G_n and G_p in this part. The numerical parameters used in this part, are provided in Table1. All the parameters in Table 1 have been selected according to valid theoretical and experimental researches [3, 7, 10].

Table1. The electrical parameters of PSC [3, 8, 11]

Parameter	TiO_2	$CH_3NH_3PbI_3$	CuSCN	Cu_2O
ε_s	9	6.5	10	3
N_c (cm^{-3})	1×10^{19}	1.66×10^{19}	1.79×10^{19}	1×10^{19}
N_D (cm^{-3})	1×10^{19}	5.41×10^{19}	2.51×10^{19}	1×10^{19}
μ_n/μ_p (cm^2/V.S)	2/1	50/50	1×10^{-4} / 0.01	3.4/3.4
χ (eV)	4	3.93	1.9	3.4
E_g (eV)	3.2	1.55	3.4	2.22
τ_n/τ_p (ns)	5/5	8/8	5/5	5/5
N_A (cm^{-3})	-	5×10^{13}	5×10^{18}	5×10^{18}
N_D (cm^{-3})	5×10^{19}	-	-	-

3 Result and discussion

The current density-voltage (*J-V*) characteristic of the perovskite solar cell in 300 K, has been shown in Fig. 3. As it is depicted, the maximum PCE ($PCE=FF*J_{sc}V_{oc}$), short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}) and fill factor ($FF=MPP/(J_{sc}V_{oc})$), have been reached to 14.32%, 18.77 (mA/cm^2), 0.98 (V) and 0.78 respectively. The PCE of the simulated PSC shows a good matching with experimental result [5]. In addition, in this work CuSCN is replaced by a Cu_2O as HTM layer [11]. The Complex refractive index of Cu_2O is taken from [12]. Electrical parameters of Cu_2O have been listed in Table1.

In Fig. 4, the current density-voltage characteristics of the simulated perovskite solar cell, (with two kinds of inorganic HTMs (Cu_2O, CuSCN)), have been shown.

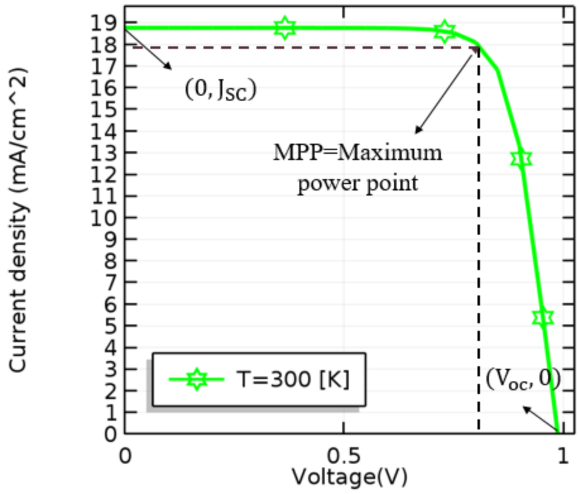

Figure 3: J–V curve of perovskite solar cell.

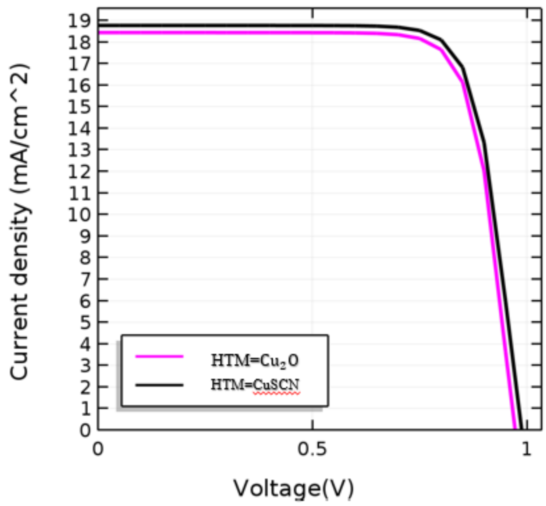

Figure 4: J-V curve of PSC with different HTM layer.

As it is shown in the results, the J_{sc} is decreased when the Cu_2O is used instead of CuSCN. This is due to total generation of carriers in perovskite layer. By using the Cu_2O layer, due to the decrease of interface reflectivity of this layer and perovskite layer for portion of input frequency range (based on material characteristic's), less amount of incident optical field is reflected to perovskite layer. As a result, the carrier generation is decreased in perovskite layer.

Another study is examination of temperature effect on solar cell performance. Fig. 6 depicts the effect of temperature (T) on *J-V* characteristics of the PSC. As it can be seen when the T increases from

280 K to 340 K, the V_{oc} decreases while the J_{sc} remains roughly intact. This is mainly because of the V_{oc} dependency to the T. This relation can be found as below [13]:

$$V_{oc} = \frac{kT}{q} \ln\left(\frac{Jsc}{J_0(T)}\right) \tag{6}$$

where k is Boltzmann constant and J_0 is a dark current density, which related to T, as below:

$$J_0 \approx B'' T^3 \exp\left(-\frac{E_{g0}}{kT}\right) \tag{7}$$

where B'' is a constant, that independent of T. So, temperature effect on the V_{oc} in solar cell is calculated as follow:

$$\frac{dV_{oc}}{dT} = -\frac{\left(V_{g0} - V_{OC}\right) + 3V_T}{T} \tag{8}$$

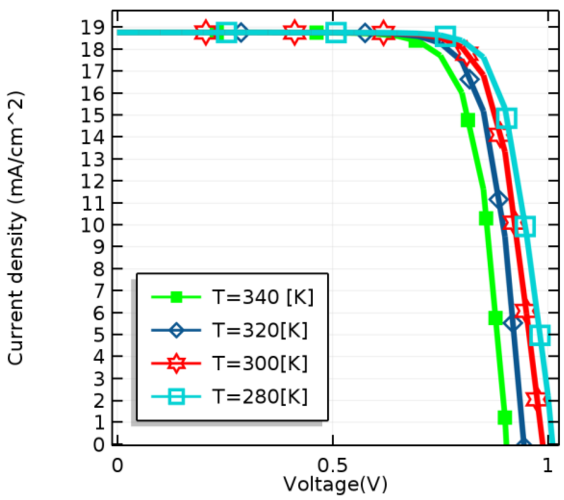

Figure 5: J-V curve of PSC as a function of temperature.

3 Conclusion

In this work, 3D FEM simulation of PSC was performed. It causes to achieve more accurate results in light propagation and electrical performance of PSCs. It was shown that, by replacing Cu_2O with CuSCN as HTM layer, the PCE is changed. In addition, as the temperature increased, due to V_{oc} reduction, the PCE of PSC is decreased.

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