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 planar 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$_2$O material instead of CuSCN), as hole transport material (HTM), has been investigated on solar cell performance. It is caused to change $J_{sc}$. 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

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

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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 MAPbX$_3$ (MA= CH$_3$NH$_3$+, 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$_3$NH$_3$PbI$_3$ 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:

$$\nabla \times (\nabla \times E) - k_0^2 \varepsilon \varepsilon_0 E = 0$$  \hspace{1cm} (1)

where, $E$ is electric field, $k_0$ is wave-vector and $\varepsilon_0$ is Complex Relative Permittivity $\varepsilon_0=n(1-i\kappa)$, which is a function of wavelength ($\lambda$).

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

$$G_{\text{photo}}(\lambda) = \frac{\varepsilon_0}{2\hbar} \left[ E \right]^2$$ \hspace{1cm} (2)

where $\hbar$ is the plank constant, $\varepsilon_0$ is the imaginary part of the $\varepsilon_0$. For $G_{\text{photo}}(\lambda)$ calculation, AM1.5G was used as the input power. The complex refractive indexes of FTO, CuSCN, TiO$_2$, CH$_3$NH$_3$PbI$_3$ and Au are taken from previously measured data [6-9]. Total generation rate ($G_{\text{tot}}$) 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:

$$\nabla (\varepsilon_0 \nabla \phi) = -\rho$$ \hspace{1cm} (3)

$$\frac{\partial n}{\partial t} = -\nabla j_n + G_n - U_n$$ \hspace{1cm} (4)

$$\frac{\partial p}{\partial t} = -\nabla j_p + G_p - U_n$$ \hspace{1cm} (5)
Another study is examination of temperature effect on solar cell performance. As it can be seen when the temperature (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]:

$$V_{oc} = \frac{kT}{q} \ln \left( \frac{J_{sc}}{J_0(T)} \right)$$  \hspace{1cm} (6)

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

$$J_0 \approx B' T^3 \exp \left(-\frac{E_g^0}{kT} \right)$$  \hspace{1cm} (7)

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

$$\frac{dV_{oc}}{dT} = - \frac{\left( V_{g0} - V_{oc} \right) + 3V_T}{T}$$  \hspace{1cm} (8)

![Figure 5: J-V curve of PSC as a function of temperature.](image)

**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 CuO 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.

**References**


