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Analysis of *I-V-T* Characteristics of $CH_3NH_3PbBr_3$ Perovskite Based Solar Cells

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The *I-V-T* characteristics of perovskite based solar cells using hybrid organic-inorganic metal halide ($CH_3NH_3PbBr_3$) as one of the material components have been studied. A numerical simulation has been performed through Solar Cell Capacitance Simulator (SCAPS-1D) software to simulate the perovskite solar cells. Poisson equation and continuity equations for the solar cells have been employed using SCAPS-1D program. The variation of the current density with voltage, current density with temperature, efficiency with defect density, and efficiency and fill factor with rise in temperature of the solar cells has been presented in this study. From the investigations, the perovskite solar cell efficiency of the order of 27.5 % has been obtained at an operating temperature of 270 K. The current density for all temperatures is constant having a value close to 25 mA/cm^2 until the supply voltage is 1.125 V. The power density increases linearly to a maximum of 27.5 mW/cm^2. The open circuit voltage and temperature are inversely proportional to each other. The obtained efficiency is 27.54 % at a defect density of 10^{15} cm^{-3}.

Keywords: SnO_2, NiO, Perovskite, Solar cells, SCAPS-1D.

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1. INTRODUCTION

Currently, perovskite solar cells have turned out to be highly promising for the future thin film photovoltaic technology. Perovskites are materials that are described by the formula ABX_3, where X is the halide anion, A is the organic ammonium, and B is the metal cation, such as lead (Pb). Perovskite based solar cells are in focus of the scientific community due to lower input costs, easy and cost-effective fabrication options, and higher output efficiency [1]. The solar cells based photovoltaic technologies are broadly classified into two different categories such as i) 1st generation PVs which are wafer-based PVs and ii) 2nd generation solar cells based on thin-film PVs [2]. The well-known examples of the 1st generation PVs are traditional crystalline silicon (c-Si) and gallium arsenide (GaAs) solar cells, which are wafer-based. Although over 90 % of the current PV market is dominated by c-Si cells, GaAs-based solar cells exhibit the highest efficiency [3, 4]. On the contrary, thin film based solar cells allow the use of extremely thin films and absorb light more efficiently than silicon based solar cells. Approximately 5 % of the total PV market is currently held by cadmium telluride (CdTe) based thin film solar cells. The successful commercialization of this technology is possible due to the high cell efficiency and module efficiency, which are reported to be more than 20 % and 17.5 %, respectively [5, 6]. Low absorption coefficient, high cost and decreased efficiency of solar cells at high temperatures are the main disadvantages of wafer-based solar cells as compared to thin-film ones [7].

Therefore, to overcome these drawbacks, an emerging thin-film PV technology based on perovskite solar cells, having the potential to extend the current cell efficiency and other performance-based limits, is in focus of the scientific community. These perovskite solar cells employ organic-inorganic metal halide based hybrids as the medium to absorb electromagnetic radiation. Due to low input material costs, high cell efficiency and inexpensive fabrication methods, these organic-inorganic metal halide based hybrids are considered promising materials for solar cell applications [8, 9]. Lead or tin halide based material, which crystallizes in the perovskite structure, is used as a light-harvesting active layer in perovskite solar cells [10]. Perovskite-based materials used in solar cells have many desired properties, such as long transport distance of electrons and holes, large absorption spectrum, fast charge separation, and longer carrier separation lifetime. As a result, these materials are very promising candidates for solid-state solar cell applications. Perovskite materials, for example, methylammonium lead halide are inexpensive to synthesize and require simple manufacturing process [11]. In 2012, Lee et al. [12] used halide perovskite materials $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$. They were apparently the first to use these materials for liquid electrolyte-based dye-sensitized solar cells.

Many characteristics of perovskite solar cells, including flexibility, lightweight and semi-transparency, have been improved to a large extent in the past few years. In addition to the above stated properties, a wide spectral absorption range, large absorption coefficient, higher carrier mobility, larger diffusion length, and longer carrier lifetime [13, 14] are also responsible for the enhanced solar cell performance. However, the current-voltage characteristics of these solar cells and per-

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formance-related degradation issues in ambient conditions have not yet been clearly studied [15].

In this research, we propose a perovskite solar cell configuration model to achieve better performance using a solar cell capacitance simulator (SCAPS-1D) [16-18]. The remaining paper is organized as follows. Section 2 presents the proposed device structure and device modeling with device parameters. Section 3 comprises of results and discussion. Finally, conclusions are given in Section 4.

2. DEVICE MODELING

These calculations were carried out by SCAPS-1D software for modeling perovskite solar cells. SCAPS-1D is a one-dimensional program and one of the renowned applications for simulation and modeling of perovskite solar cells. This software was developed by the Department of Electronics and Information Systems (ELIS), University of Ghent, Belgium. SCAPS-1D software was designed to simulate electrical characteristics at different operating temperatures.

SCAPS-1D is based on solving basic semiconductor equations, including Poisson's equation (1) and continuity equations (2) and (3):

$$\begin{cases} \dfrac{\partial^2}{\partial x^2}\phi(x) = \dfrac{q}{\varepsilon}\left[n(x) - p(x) - N_D^+(x) + N_A^-(x) - p_t(x) + n_t(x) \right] \\ \dfrac{\partial J_n}{\partial x} = G - R_n \\ \dfrac{\partial J_p}{\partial x} = G - R_p \end{cases} \tag{1-3}$$

The electron and hole current densities are given by

$$\begin{cases} J_n = qn\mu_n \dfrac{\partial \phi}{\partial x} + qD_n \dfrac{\partial n}{\partial x} \\ J_p = -qp\mu_p \dfrac{\partial \phi}{\partial x} + qD_p \dfrac{\partial p}{\partial x} \end{cases},$$

where φ is the electrostatic potential, q is the electric charge, ε is the permittivity of free space, n is the concentration of free electrons, p is the concentration of free holes, N_D^+ are the ionized donors, N_A^- are the ionized acceptors, p_t is the density of trapped holes, n_t is the density of trapped electrons, G is the generation rate, R is the recombination rate, D_n is the electron diffusion coefficient, D_p is the hole diffusion coefficient.

Poisson's equation relates the electrostatic potential to charge, whereas the continuity equations for holes and electrons include field drift due to the potential gradient. At the interfaces and contacts, appropriate boundary conditions are used to get coupled differential equations. These equations are solved to determine solar cell device parameters.

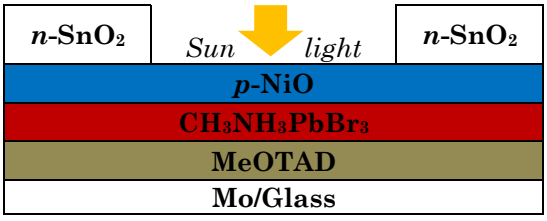

Fig. 1 – Schematic structure of a perovskite solar cell

Table 1 – Parameters used for the simulation

Parameters	SnO_2	NiO	$CH_3NH_3PbBr_3$	MeOTAD
Thickness (μm)	0.06	0.08	0.1	1.5
E_g (eV)	3.6	3.9	2.2	2.99
N_a (cm^{-3})	10^{10}	10^{19}	10^{10}	10^{19}
N_d (cm^{-3})	10^{19}	10^{10}	10^{19}	10^{7}

Fig. 1 represents the schematic diagram of a perovskite solar cell. The material parameters of each layer employed for the simulation are shown in Table 1.

3. RESULTS AND DISCUSSION

Fig. 2 illustrates the *J-V* characteristics of the perovskite solar cell presented in Fig. 1. It shows the variation of current density as a function of applied voltage at different temperatures between 270-320 K for every 10 K. Initially, the current density for all temperatures is constant and has a value close to 25 mA/cm² until the supply voltage is 1.125 V. Thereafter, the current density suddenly decreases. The voltage corresponding to the onset of a sharp decrease in the current density deceases linearly with increasing temperature.

On the other hand, Fig. 3 shows the variation of power generated by the perovskite solar cell at 270 K as a function of electric field. We observe that the power density increases linearly to a maximum of about 27.5 mW/cm². However, the series resistance of the perovskite solar cell tends to decrease the Fill Factor (FF) significantly [19].

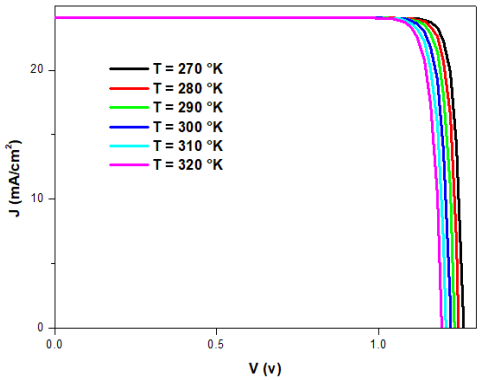

Fig. 2 – *J-V* characteristics of the perovskite solar cell

In addition, Fig. 4 illustrates the variation of open-

circuit voltage and short-circuit photocurrent density with temperature. Small variation in the photocurrent increases exponentially with increasing temperature and vice versa. On the other hand, open-circuit voltage and temperature are inversely proportional to each other. The open-circuit voltage decreases linearly with increasing temperature and vice versa.

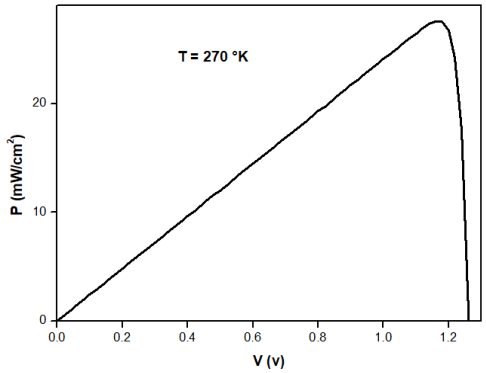

Fig. 3 – *P*(*V*) characteristic of the perovskite solar cell at 270 K

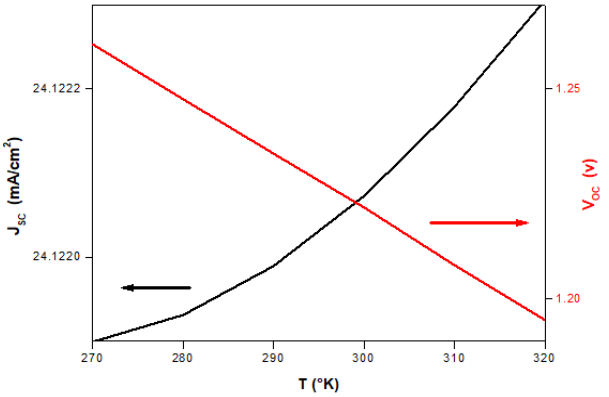

Fig. 4 – Influence of temperature on short-circuit photocurrent density and open-circuit voltage

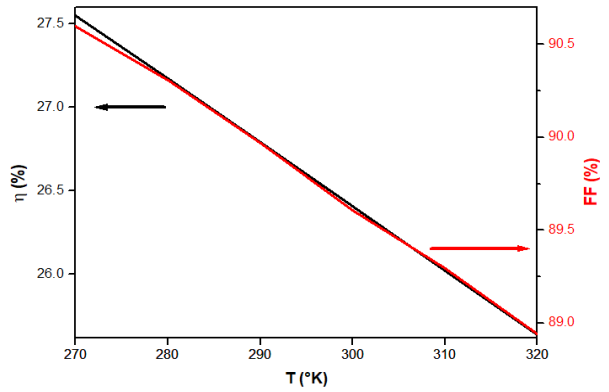

Fig. 5 – Effect of temperature on the efficiency and FF

The influence of temperature on the efficiency and Fill Factor (FF) of the perovskite solar cell is shown in Fig. 5. It can be seen that both the solar cell efficiency and FF are inversely proportional to temperature. The drop in FF also reduces the maximum power energy [20]. At 270 K, the proposed perovskite solar cell achieves the efficiency of 27.6 % and FF of 27.5 %. With increasing temperature, both parameters are reduced significantly.

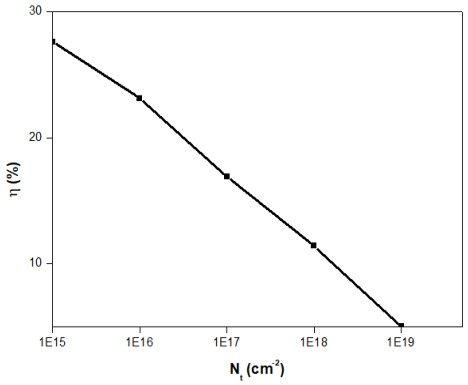

Fig. 6 – Variation of efficiency with defect density

The defect density plays an important role in boosting the device performance. A higher defect density in the absorber film is due to higher recombination because of the formation of holes, a higher degree of degradation of the layer, and also a decrease in the performance of the device [21]. To optimize the defect density in the absorber, simulation was done by changing the defect density at 270 K from 10^{15} to 10^{19} cm^{-3}. As shown in Fig. 6, the obtained efficiency is 27.54 % at a defect density of 10^{15} cm^{-3}.

4. CONCLUSIONS

The *I-V-T* characteristic of the perovskite based solar cell shows that the current density remains constant with voltage and decreases linearly with an increase in temperature in the range studied. The open-circuit voltage increases non-linearly with temperature, whereas the efficiency and fill factor decrease with the rise in temperature of the solar cell. From the investigations, the perovskite solar cell efficiency of the order of 27.5 % is obtained at an operating temperature of 270 K. The defect density in the absorber should be maintained up to order of 10^{15} cm^{-3}.

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Аналіз характеристик *I-V-T* сонячних елементів на основі перовскіту $CH_3NH_3PbBr_3$

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Досліджено характеристики *I-V-T* сонячних елементів на основі перовскіту з використанням гібридного органічно-неорганічного галогеніду металу ($CH_3NH_3PbBr_3$) як одного з компонентів матеріалу. Чисельне моделювання було виконано за допомогою програмного забезпечення SCAPS-1D для моделювання перовскітних сонячних елементів. Рівняння Пуассона та рівняння безперервності для сонячних елементів були використані за допомогою програми SCAPS-1D. У дослідженні представлено залежності густини струму від напруги, густини струму від температури, коефіцієнта корисної дії від густини дефектів, а також коефіцієнта корисної дії та коефіцієнта заповнення від температури сонячних елементів. З досліджень було отримано коефіцієнт корисної дії перовскітних сонячних елементів близько 27,5 % при робочій температурі 270 К. Густина струму для всіх температур є постійною і має значення, близьке до 25 мА/см^2, для напруги живлення 1,125 В. Густина потужності лінійно зростає до максимуму 27,5 мВт/см^2. Напруга холостого ходу і температура обернено пропорційні одна одній. Отримане значення коефіцієнта корисної дії становить 27,54 % при густині дефектів 10^{15} см$^{-3}$.

Ключові слова: SnO_2, NiO, Перовскіт, Сонячні елементи, SCAPS-1D.