Study of the effect of the thickness of the photosensitive layer of perovskite on its efficiency using SCAPS-1D software

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Abstract. Photovoltaic cells are the best way to convert solar energy into electrical energy by absorbing photons emitted by the sun. This paper presents the results of studies of the effect of the thickness of the absorbing layer of perovskite on the quantum efficiency of the solar cell, as well as on its efficiency. These results were obtained by modelling in the software product SCAPS-1D. Perovskite photovoltaic is getting to be a distinctly predominant option for the conventional solar cells achieving maximum efficiency of 22.1% and more. This work is concerned about the design and analyses of lead-based perovskite solar cell model with the architecture of TiO2/CH3NH3PbI3/spiro-OMeTAD. The analysis of solar cell architecture is done using the Solar Cell Capacitance Simulator (SCAPS). It is a computer-based software tool and is well adapted for the analyses of homo and heterojunctions, multi-junctions and Schottky barrier photovoltaic devices. This software tool runs and simulates based on the Poisson’s and continuity equation of electrons and holes. For this model, it is used to optimize the various parameters such as thickness, the defect density of absorber layer, doping concentrations (ND and NA) of Electron Transport Material (ETM) and Hole Transport Material (HTM)

1. Introduction

The use of solar energy is recognized as a promising way to solve the global energy crisis. In recent decades, photosensitive films based on perovskite have shown promise for creating highly efficient and inexpensive solar cells. The thickness of the perovskite film is one of the key parameters for achieving high efficiency of the solar cell. The thickness should be sufficient to absorb a large number of photons but too thick a layer of perovskite creates more recombination centers and prevents the transfer of photogenerated charge carriers due to a decrease in the electric field in the perovskite, which reduces the characteristics of the solar cell. The optimal thickness should be consistent with the perovskite thickness and the diffusion length (lifetime) of the charge carriers [1]. The main stage of optimizing the structure and improving the characteristics of solar cells is modeling. This work is devoted to modeling and research of lead-based perovskite solar cells using SCAPS (Solar Cell Capacity Simulator) software. SCAPS is a program for numerical simulation of solar cells developed at the Department of electronics.
and information systems (ELIS) of the University of Ghent (Belgium) [2]. Promising for photovoltaic applications, ORGANOMETALLIC perovskite is a material with a crystal structure (ABX₃) similar to the crystal lattice of calcium titanate (CaTiO₃). The main advantages of lead methylammonium iodide (CH₃NH₃PbI₃) perovskites are the absence of energy-intensive and complex technological processes when applied to various substrates (crystallization temperature of 100-150 °C), as well as their characteristic forbidden zone (1.5-2.3 eV) with direct transitions, high mobility of charge carriers (0.1-10 cm²V⁻¹C⁻¹), relatively large diffusion length (0.1-1.5 microns) and high absorption coefficient (more than 5×10⁴ cm⁻¹) [3]. Modeling is an important and necessary stage in the development and manufacture of new semiconductor devices, in particular solar cells, which reduces the cost of conducting experimental research and optimizing parameters.

2. Experimental part
The output characteristics of a perovskite solar cell depend significantly on the thickness of the absorbing layer of perovskite. The solar cell model in the SCAPS program consisted of TiO₂/CH₃NH₃PbI₃/spiro-OMeTAD layers, where TiO₂ is a conductor for electrons, CH₃NH₃PbI₃ is a photosensitive (absorbing) layer, and spiro-OMeTAD is a conductor for holes [4]. The thickness of TiO₂ and spiro-OMeTAD layers were set constant, and the thickness of the photosensitive layer varied from 100 to 500 nm for the first experiment and from 100 to 900 nm for the second experiment, respectively. This model is calculated based on the diffusion-drift system of semiconductor equations, which includes stationary differential continuity equations for determining electron and hole concentrations, as well as the Poisson equation for calculating the potential in perovskite [5]:

\[
D_e \frac{d^2n(x)}{dx^2} + \frac{\mu_e}{\epsilon_0} \left( \frac{dn(x)}{dx} \right) \frac{d\phi(x)}{dx} + n(x) \left( \frac{d^2\phi(x)}{dx^2} \right) + G(x) - R(x) = 0,
\]

\[
D_h^+ \frac{d^2p(x)}{dx^2} + \frac{\mu_h^+}{\epsilon_0} \left( \frac{dp(x)}{dx} \right) \frac{d\phi(x)}{dx} + p(x) \left( \frac{d^2\phi(x)}{dx^2} \right) + G(x) - R(x) = 0,
\]

\[
\frac{d^2\phi(x)}{dx^2} = \frac{q(n(x)-p(x))}{\epsilon_0},
\]

where \( n \) and \( p \) - the concentrations of electrons and holes; \( D_e \) and \( D_h^+ \) - the diffusion coefficient of electrons and holes; \( \mu_e \) and \( \mu_h^+ \) - the mobility of electrons and holes; \( \phi \) - the electrostatic potential; \( q \) - the elementary charge; \( \epsilon_0 \) - the relative dielectric permittivity; \( \epsilon_0 \) - the electric constant, \( G \) - the optical generation rate of electron-hole pairs; \( R \) - the recombination rate of electron-hole pairs. The rate of charge carrier generation was determined in the spectral range of perovskite absorption based on the boogek-Lambert law and the approximation of the solar spectrum AM1.5 by the spectrum of thermal radiation at a temperature of 300 K (Planck's formula) [5, 7]:

\[
G = \eta \alpha (1 - T) \Phi e^{-\alpha x},
\]

where \( \eta \) - the photon generation coefficient of electron-hole pairs; \( \alpha \) - the perovskite absorption coefficient; \( T \) - the reflection coefficient from the front surface; \( \Phi \) - the photon flux density in the perovskite absorption spectral range:

\[
\Phi = \int_{200}^{800} K \left( \frac{R_S}{r_0} \right)^2 \left( \frac{2\pi c}{\lambda^2} \right) \frac{F}{K e^{\lambda xx - \lambda x}} \, d\lambda,
\]

\( \lambda \) - the wavelength; \( h \) - Planck's constant; \( c \) - the speed of light in a vacuum; \( F \) - the shading coefficient; \( R_S \) - the radius of the Sun; \( T \) - the temperature of the Sun; \( K \) - the coefficient reflecting the influence of the earth's atmospheric mass on the solar radiation power density for the AM1.5 spectrum.
Figure 1. Model of study of the Sollar element.

The parameters obtained from the articles [6-9] were used for modeling. Table 1 shows the initial parameters of each of the layers of the studied solar cell, which were taken into account in the modeling process.

![Figure 2](image)

Figure 2. Zone diagram of the studied model of a perovskite solar cell.

Table 1. Initial parameters of the solar cell under study.

| Parameters                                | HTM   | \(\text{CH}_3\text{NH}_3\text{PbI}_3\) | \(\text{TiO}_2\) |
|-------------------------------------------|-------|--------------------------------------|------------------|
| Thickness (nm)                            | 350   | variable                             | 30               |
| Bandgap (eV)                              | 3     | 1.55                                 | 3.2              |
| Electron affinity (eV)                    | 2.45  | 4.5                                  | 4.26             |
| Dielectric permittivity (relative)         | 3     | 10                                   | 9                |
| CB effective density of states (1/cm\(^3\)) | 2.2\(\times10^{18}\) | 2.2\(\times10^{18}\) | 2\(\times10^{18}\) |
| VB effective density of states (1/cm\(^3\)) | 1.8\(\times10^{19}\) | 1.8\(\times10^{19}\) | 1.8\(\times10^{19}\) |
| Electron thermal velocity (cm/s)          | 1\(\times10^{7}\) | 3\(\times10^{7}\) | 1\(\times10^{7}\) |
| Hole thermal velocity (cm/s)              | 1\(\times10^{7}\) | 3\(\times10^{7}\) | 1\(\times10^{7}\) |
| Electron mobility (cm\(^2\)/Vs)          | 2\(\times10^{-4}\) | 1.6\(\times10^{1}\) | 2\(\times10^{1}\) |
The direction of solar radiation was modeled from the TiO₂ side. The simulation process took place at a set temperature of 300 K. Figure 2 shows the dependence of the quantum efficiency of the solar cell on the thickness of the perovskite layer. Quantum efficiency describes the ratio of the number of photons whose absorption led to the generation of electron-hole pairs to the total number of photons absorbed. As a result of the study, it was found that an increase in the thickness of the perovskite layer causes a significant increase in quantum efficiency. When the thickness of the perovskite layer increases from 100 to 500 nm, the quantum efficiency increases almost twice – from 45 to 90 %. This is due to the fact that more photons will be absorbed by the perovskite layer, which will lead to an increase in the generation of electron-hole pairs [5].

![Figure 3. Dependence of the quantum efficiency of the solar cell on the thickness of the perovskite layer.](image)

**Table 2.** Output characteristics of the studied SE model in the range of 100-500 nm.

| QE (%) | Thickness (nm) |
|--------|----------------|
| 43     | 100            |
| 59     | 150            |
| 72     | 200            |
| 78     | 250            |
| 83     | 300            |
| 89     | 400            |
| 89     | 500            |
Figure 3 also shows that when the perovskite layer is about 400 nm thick, the quantum efficiency of the solar cell reaches a maximum of 89%. Therefore, a further increase in the perovskite layer does not lead to an increase in quantum efficiency.

Further, the estimation of the change in the efficiency of the solar cell with an increase in the thickness of the perovskite layer was made. The thickness of the photosensitive layer varied from 100 to 900 nm.

![Graph showing efficiency vs. thickness](image)

**Figure 4.** Dependence of efficiency on the thickness of the photosensitive layer.

**Table 3.** Output characteristics of the studied SE model in the range of 100-900 nm.

| Efficiency (%) | Thickness (nm) |
|---------------|----------------|
| 8.5           | 100            |
| 15.9          | 250            |
| 17.9          | 400            |
| 19.5          | 550            |
| 18.5          | 700            |
| 16.9          | 900            |

As a result, it was found that when the thickness of the photosensitive layer increases from 100 to 900 nm, the efficiency of the solar cell increases more than twice - from 8.5% to 19.5%. Comparison of the first and second graphs shows that an increase in quantum efficiency plays a significant role in increasing the efficiency at the thickness of the photosensitive layer up to 400 nm. With increasing thickness of the photosensitive layer is above 400 nm the increase in efficiency occurs only slightly and a decrease in efficiency when a thicker film, which is due to increased recombination losses (decreasing the electric field in perovskite promotes separation of photogenerated electron-hole pairs).
3. Conclusion
Thus, using the developed mathematical model of the solar cell based on perovskite, it was shown that an increase in the photosensitive layer leads to greater absorption of the number of photons and the generation of electron-hole pairs. The presence of a maximum is due to the fact that as the thickness of the perovskite film increases, the solar cell's photocurrent increases, which goes out to saturation, while the photon voltage decreases with increasing thickness due to an increase in the recombination rate. In this case, by increasing the thickness of the photosensitive layer from 100 to 550 nm, the efficiency increases more than twice - from 8.5% to 19.5%.

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References
[1] Malyukov S P, Saenko A V and Ivanova A V 2016 Numerical simulation of perovskite solar cells with a flat structure IOP Conference series: Material Science and Engineering 151 2016 012033
[2] Electronics and Information Systems (ELIS) (Dept: University of Ghent) http://scaps.elis.ugent.be/ (accessed: 10.02.2020).
[3] Gratzel M 2014 Nature Materials 13 838
[4] Sinshu sun, Reza Asadpour, Wanyi ne, et al. 2015 IEEE Journal of Photovoltaics 5 1389
[5] Abdelkader H, Ahmed Khalil Le K, Abdallah R, Muslem Ben, Abderrahman K Imad K 2019 Modeling and optimization of CH_3 NH_3 PbI_3 based on inverted planar heterojunction of solar cells using SCAPS software Journal. from Energetica (IJECA) 4(1) 56-59
[6] Du H J and Zhu J Z 2016 The device for simulation of lead-free status CH3NH3SnI3 perovskite solar cells with high efficiency Chinese Physics B 25 108802
[7] Mandadapu U, Vedanayakam S V and Thyagarajan K 2017 Modeling and analysis of lead-based perovskite solar cells using SCAPS-1D Indian Journal of Science and Technology 10(11) 0974-6846
[8] Ameri M, Mohajerani E and Aparcana M 2019 Investigation of this case the invisible relationship between grain size, ion defects, device physics, and performance of perovskite solar cells Journal of Physics D Applied physics 52 125
[9] Thakur N, Mehra R and Devi K 2018 Efficient design Perovskite solar cell using parametric grading of mixed perovskite Halide and copper iodid. Journal of Electronic Materials 47 6935–6942