GPVDM simulation of layer thickness effect on power conversion efficiency of CH$_3$NH$_3$PbI$_3$ based planar heterojunction solar cell

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Abstract – Perovskite-based solar cell technologies have been a very attractive area of research in recent years. Organic-inorganic perovskite materials are in an increased evolution in power conversion efficiency. Inorganic materials have been tested at the laboratory level but their power conversion efficiency is still limited. In this paper, we used the GPVDM software to study the effect of some parameters on power conversion efficiency in a planar heterojunction solar cell based on CH$_3$NH$_3$PbI$_3$ as an absorbing layer. The modifications were made by considering layers of perovskite without defects. The results show that the efficiency of the power conversion can be improved by adjusting layer thickness; in our case power conversion efficiency was increased from 9.96 % to 12.9 %.

Keywords: Perovskite, MAPbI$_3$, PCE, GPVDM Software, layer thickness

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I. Introduction

The very peculiar structure of perovskites is at the origin of many researches in various fields of physics and their applications. It was discovered in 1940 that synthetic ceramics of perovskite structure such as barium titanate (BaTiO$_3$) had remarkable piezoelectric properties, that is to say that they were electrically polarized easily under the action of mechanical stresses. Perovskite-type single crystals have been more recently manufactured with even more interesting piezoelectric properties.

The research in laboratories on hybrid organic-inorganic perovskites has become very intensive. This new technology of perovskite solar cells has seen a rapid progression and each time new percentage of power conversion efficiency that appear. To see the surprising progression of this area reminds that in 2009 a study was made on a cell based on CH$_3$NH$_3$PbBr$_3$ with a high photovoltage of 0.96 V and the value of the efficiency was 3.8% [1]. After two years in 2011, a Perovskite cell of size 2-3 nm (CH$_3$NH$_3$PbI$_3$) nanocrystal gave a solar-electric conversion efficiency of 6.54% [2]. During the year 2013, energy conversion efficiencies reached an astounding 16.2% [3]. In the same year, an optimization of the TiO$_2$ layer treatment conditions, yields a PCE of 19.3% [4, 6]. Almost five years of research, it became between 22.1 and 22.6 % [7]

Different parameters can increase PCE in perovskite based solar cells; one of them is layer thickness of different layers. In the present paper we used GPVDM which is a powerful software simulation for photovoltaics, where we investigated effect of different layer thickness on power conversion efficiency of a planar heterojunction solar cell using CH$_3$NH$_3$PbI$_3$ as absorber layer.

II. Device simulation parameters

General-Purpose Photovoltaic Device Model (GPVDM) is free general purpose software for solar cell simulation based on solving Poisson equation (1) and the bipolar drift diffusion equations (2,3) and the carrier continuity equations (4,5) in 1D and time domain.

$$\frac{d}{dx} \varepsilon_0 E_x - \frac{d\phi}{dx} = q(n-p) \quad (1)$$

$$J_n = q \mu_n \frac{\partial E}{\partial x} + q D_n \frac{\partial n}{\partial x} \quad (2)$$

$$J_p = q \mu_p \frac{\partial E}{\partial x} - q D_p \frac{\partial p}{\partial x} \quad (3)$$

$$\frac{\partial J_n}{\partial x} = q \left( R_n - G + \frac{\partial n}{\partial x} \right) \quad (4)$$
\[
\frac{\partial J_p}{\partial x} = -q \left( R_p - G + \frac{\partial p}{\partial t} \right) 
\]  \hspace{1cm} (5)

More detail on above equation resolving and device modeling can be found in more detail in \[8\text{-}11\]. GPVDM software graphical interface is shown in Figure 1.

In Figure 2 is shown the planar heterojunction architecture of a CH$_3$NH$_3$PbI$_3$ based solar sell. The layer configuration adopted in this simulation is Glass/TCO/ETM/CH$_3$NH$_3$PbI$_3$/HTM/Silver where ETM layer is the TiO$_2$ and the HTM layer is the spiro-OMeTAD. In Table 1 is shown initial parameters that were carefully picked from practical and theoretical references \[12\text{-}21\]. Perovskite electrical and optical parameters are set from \[16\] and from GPVDM software database based on \[22\]. Glass layer and silver layer thickness are taken 6$\times$10$^{-8}$ m and 2$\times$10$^{-7}$ m respectively.

Our simulation is based on study of effects of different layer thickness on power conversion efficiency. Initial layer thickness given in Table 1 yields the J-V characteristic curve shown in Figure 3, in which power conversion efficiency PCE is 9.96 %, fill factor is 75.86 %, Open-circuit voltage $V_{oc}$ is 0.47 V and short-circuit density of current is -277 A/m$^2$.

![Figure 1. GPVDM Home window.](image1)

![Figure 2. Planar heterojunction architecture of the studied solar cell](image2)

| Parameters | FTO | TiO$_2$ | CH$_3$NH$_3$PbI$_3$ | spiro-OMeTAD |
|------------|-----|---------|---------------------|--------------|
| Layer thickness (m) | 1e-7 (variable) | 2.5e-8 (variable) | 1e-7 (variable) | 1e-7 (variable) |
| Relative permittivity $\varepsilon_r$ | 3 | 9 | 3 | 3 |
| Band gap energy (eV) | 0 | 3.2 | 2.1 | 3.17 |
| Electron affinity (eV) | 4.7 | 4.26 | 3.7 | 2.05 |
| Electron mobility (m$^2$/V.s) | 6.86e-07 | 20e-4 | 6.86e-07 | 2e-08 |
| Hole mobility (m$^2$/V.s) | 3.75e-02 | 10e-4 | 3.75e-02 | 2e-08 |
| Donor concentration (m$^{-3}$) | 5e26 | 1e22 | 5e26 | 0 |
| Acceptor concentration (m$^{-3}$) | 5e26 | 0 | 5e26 | 2e25 |

Table 1. Simulation parameters
III. Results and discussion

Optimization method used in our simulation is to fix all parameters and modify one by one until we have the parameters that gives maximal PCE. In Figure 4 is presented the curve of effect of perovskite layer thickness on PCE.

From Figure 4 we can note that a perovskite layer thickness of $2 \times 10^{-7}$ m gives the maximal value of PCE which is 12.83 %, with a fill factor of 74.79 %, an open-circuit voltage of 0.47 V and a short-circuit density of current of -370 A/m$^2$.

We fix the CH$_3$NH$_3$PbI$_3$ layer thickness on $2 \times 10^{-7}$ m and we change the FTO layer thickness to obtain curve in Figure 5.

Curve of Figure 7 shows that Maximal PCE of 12.9 % is obtained in TiO$_2$ layer thickness of $2.5 \times 10^{-8}$ m, where fill factor is 74.79 %, open-circuit voltage is 0.47 V and short-circuit density of current is -372 A/m$^2$.

In Figure 6 we can note that the maximal PCE is 12.90 % in the spiro-OMeTAD layer thickness of $10^{-7}$ m with a fill factor of 74.79 %, an open-circuit voltage of 0.47 V and a short-circuit density of current of -372 A/m$^2$.

When spiro-OMeTAD layer thickness is set to $10^{-7}$ m and changing of TiO$_2$ layer thickness we obtained curve in Figure 7.
In Figure 8 above we can see J-V characteristic of the studied solar cell with optimized parameters.

IV. Conclusion

Perovskite power conversion efficiency was analyzed using the GPVDM solar cell software simulation. Results indicate that a good choice of layer thickness of different materials used in the solar cell increases considerably the PCE ratio. From Simulation results is found that an improvement of 2.94 % is made by setting layer thickness of FTO to 4×10^{-8} m, of TiO_2 to 2.5×10^{-8} m, of Perovskite to 2×10^{-7} m and of spiro-OMeTAD to 10^{-7} m. Further PCE enhancements can be done by changing layer structure and materials.

V. Nomenclature

\( \varepsilon_0 \) is the permittivity of free space  
\( \varepsilon_r \) is the relative permittivity  
\( \phi \) is the voltage profile  
\( q \) is the elementary charge on an electron  
\( n \) is the free electron concentration  
\( p \) is the free hole concentration  
\( J_{ne} \) is the electron current flux density  
\( J_{nh} \) is the hole flux density  
\( \mu_e \) is the electron mobility  
\( \mu_h \) is the hole mobility  
\( E_e \) is the free electron mobility edge  
\( E_h \) is the free hole mobility edge  
\( D_e \) is the electron diffusion coefficient  
\( D_h \) is the hole diffusion coefficient  
\( R_n \) is the net recombination rate for electrons  
\( R_p \) is the net recombination rate for holes  
\( G \) is the free carrier generation rate

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