

Influence of Electron Transport Layer and Hole Transport Layer on the Performance of Perovskite-based Solar Cells (PSCs)

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Abstract Photovoltaic solar cells are currently the focus of many research projects to produce low-cost, high-quality solar cells. With this in mind, third-generation solar cells are positioned as an alternative to conventional solar cells. Perovskite-based solar cells are the focus of much interest because of their exciting optoelectronic properties. Knowledge of the properties of this cell is necessary to design high-quality solar cells. Our study is based on the influence of the electron (TiO₂) and hole (Spiro-OMeTAD) transport layers on the performance of the perovskite solar cell (PSCs). For this research, we used the Solar Cell Capacitance Simulator in 1 Dimension (SCAPS-1D) software, developed by the University of Gent in Belgium, to carry out numerical simulations on a perovskite solar cell. The calculation methodology is based on the finite difference method and integrates the transport properties, Poisson, and continuity equations, using predefined boundary conditions. Through this simulation, we studied the influence of the thickness variation and the electron transport layer's doping. In addition, we examined the doping and the mobility of the holes in the 2,2',7,7' tetrakis (N, N-di-p-methoxyphenylamine)-9,9'-spirobifluorene (Spiro-OMeTAD) layer on the performance of perovskite solar cell (PSCs). Good stabilities are observed when the doping of the electron transport layer is of the order of 10¹⁴cm⁻³ for an ultra-thin thickness and optimum values are obtained for a doping of 10²⁰cm⁻³ and a mobility greater than 10⁻³cm²/Vs in the HTL layer.

Keywords: Perovskite, Mobility, Doping, Defect density

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1. Introduction

The performance of the perovskite solar cell (PSCs) is generally based on several parameters, including the impact of window layers such as titanium dioxide (TiO₂) and 2,2',7,7' tetrakis (N, N-di-p-methoxyphenylamine)-9,9'-spirobifluorene (Spiro-OMeTAD). TiO₂ is a semiconductor material used as a transparent mesoporous layer for transporting electrons in (PSCs) [1]. It is a material of great interest due to its non-toxic nature, unique optical and electrical properties, low cost, high chemical stability, and stability against corrosion [2]. Spiro-OMeTAD is used to transport holes in perovskite-based solar cells [3]. Initially used in DSSCs by Michael Grätzel's team in 1998 [4], Spiro-OMeTAD is still the hole-conducting layer in perovskite photovoltaic cells. Despite the significant advances made over the last few

decades in developing TiO₂ and Spiro-OMeTAD-based nanomaterials, knowledge of the properties of these two layers remains a major challenge in the scientific field. This paper explores the impact of certain parameters of these two layers on the performance of the perovskite solar cell. To do this, we used the numerical simulation software Solar Cell Capacitance Simulator in 1 Dimension (SCAPS 1-D) [5], with well-defined input parameters to conduct the simulation. The methodology used for the simulation with SCAPS 1-D is based on the finite difference method with the solution of equations with well-defined boundary conditions. In this paper, we will first evaluate the impact of varying the thickness of the TiO₂ layer, the influence of defect density in the TiO₂ layer as a function of thickness, and the impact of TiO₂ layer doping and mobility on cell stability. Secondly, an assessment will be made of the impact of the doping and thickness of the Spiro-OMeTAD layer, the impact of mobility and doping, and, finally, the impact of mobility

and thickness on the stability of the perovskite solar cell. Good performances are observed with doping the TiO_2 layer of the order of 10^{14} cm^{-3} for an ultra-thin thickness, while optimum values are achieved with doping of 10^{20} cm^{-3} and mobility greater than $10^{-3} \text{ cm}^2/\text{Vs}$ in the TiO_2 layer.

2. Materials and Methods

2.1. The Structure of the Solar Cell Studied

Figure 1 shows the structure of a perovskite-based solar cell. It comprises a glass substrate to which FTO-doped tin oxide is applied. Titanium dioxide is deposited on top of the **Fluorine-doped Tin Oxide** (FTO) and acts as an electron transport layer (ETL). The active layer is made of perovskite material. To optimize hole transport, a layer of spiro-OMeTAD (HTL) is inserted between the gold electrode and the active layer.

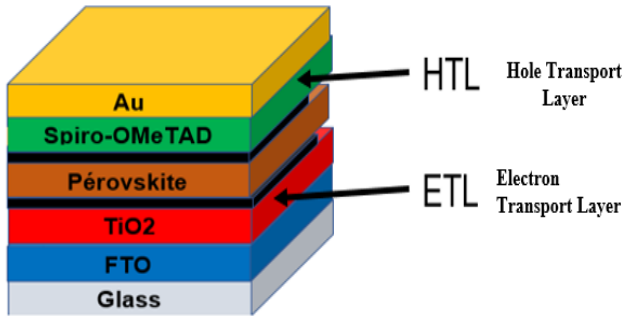


Figure 1. Structure of a perovskite cell

2.2. Fundamental Equations for Simulation Software

Several years of research into the physics of semiconductor-based devices have led to the development of mathematical models. These models are essentially based on solving the Poisson and continuity equations for electrons and holes.

2.3. Poisson Equation

$$\text{div } \vec{E} = \frac{\rho}{\epsilon} \quad (1)$$

E: Represents the electric field

ϵ is the dielectric permittivity, and ρ is the volume density of the free charges

2.4. Continuity Equations

$$\nabla J_n = q[R(x) - G(x)] + q \frac{\partial n}{\partial t} \quad (2)$$

$$\nabla J_p = q[R(x) - G(x)] + q \frac{\partial p}{\partial t} \quad (3)$$

$R(x)$ and $G(x)$ are the electron and hole recombination rates respectively; J_n and J_p are the electron and hole current densities

3. Results and Discussion

The results of the numerical simulation of a perovskite solar cell using the SCAPS-1D software allowed us to determine the impact of the electron transport layer and hole transport layers on the performance of the perovskite solar cell (PSCs). These parameters include variation in titanium dioxide (TiO_2) layer thickness, the defect density in the TiO_2 layer, and as a function of thickness, TiO_2 layer doping and mobility, the influence of 2,2',7,7'-tetrakis (N, N-di-p-methoxyphenylamine)-9,9'-spirobifluorene (Spiro-OMeTAD) layer doping and thickness, influence of mobility and doping, and influence of mobility and thickness on cell performance. The optimum parameters obtained could be used to manufacture perovskite-based solar cells that perform better than conventional solar cells.

3.1. Influence of TiO_2 Layer Thickness Variation on Electrical Parameters

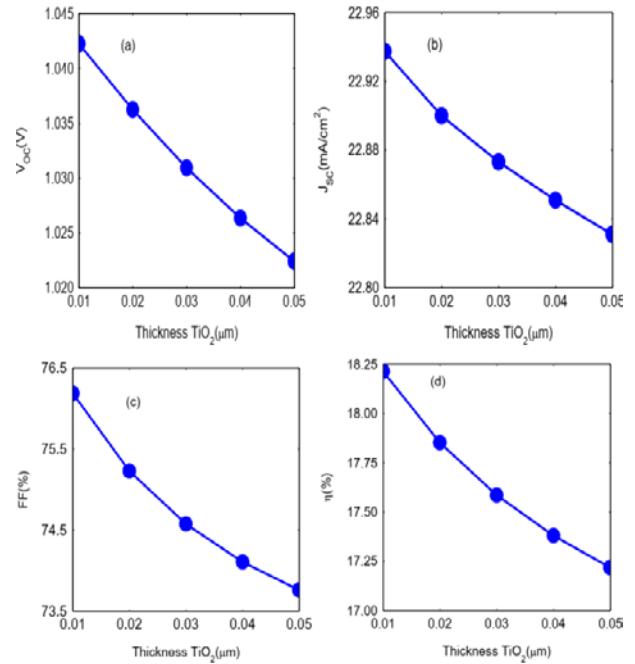


Figure 2. Influence of TiO_2 layer thickness on electrical parameters

Figure 2 illustrates the effect of the thickness of the TiO_2 window layer on the electrical parameters of a perovskite solar cell. The data indicate that varying the thickness of the electron transport layer significantly influences the solar cell's performance, with all electrical parameters decreasing as the thickness increases. This decline in performance may be attributed to the composition of the perovskite material, the properties of the other underlying cell layers, and the manufacturing conditions [6]. At the open-circuit voltage (V_{oc}) level, the thickness of the TiO_2 layer impacts the Fermi level and the contact barrier between the perovskite and the TiO_2 electrode. Excessive thickness can cause a shift in the Fermi levels, reducing the Conversely, a layer that is too thin can lead to current leakage, further decreasing the voltage (V_{oc}) [7]. For the short-circuit current density (J_{sc}) the TiO_2 layer thickness affects the amount of light

absorbed by the perovskite. An excessively thick layer may absorb a significant portion of the incident light, reducing (J_{SC}). On the other hand, a layer that is too thin may allow excessive light transmission, also negatively impacting the current density [8]. Regarding the fill factor (FF), which characterizes the efficiency of extracting maximum power from the incident light, the TiO_2 layer thickness can affect the FF by promoting recombination losses and increasing the cell's internal resistance. Finally, concerning overall efficiency, a TiO_2 layer that is too thin reduces the distance electrons must travel to reach the electrode, potentially minimizing recombination losses and improving energy conversion efficiency.

3.2. Influence of Defect Density in the TiO_2 Layer and as a Function of Thickness

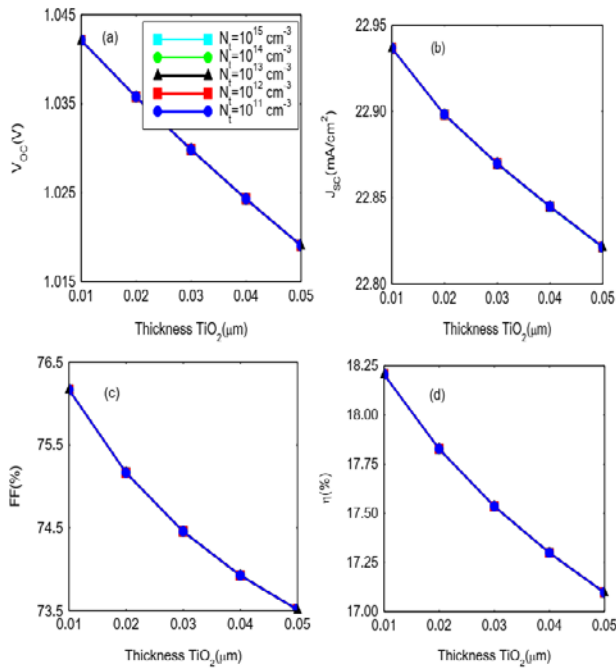


Figure 3. Influence of defect density in the TiO_2 layer and thickness on electrical parameters

Figure 3 illustrates the variation in defect density and the thickness of the TiO_2 layer on the electrical parameters of a perovskite solar cell. It shows similar trends to those observed in Figure 2, where all parameters decrease as the thickness increases. This observation suggests that variations in defect density within the transport layer may not significantly affect the electrical parameters [4]. However, this interpretation may not be entirely accurate. In our study, this trend could be explained by the fact that a high defect density in the TiO_2 layer leads to increased charge carrier recombination, which consequently reduces the open-circuit voltage V_{OC} [9]. Additionally, a thicker TiO_2 layer increases the distance that charge carriers must travel to reach the contacts, further exacerbating recombination losses and reducing V_{OC} . The optimal thickness of the TiO_2 layer depends on several factors, including charge carrier mobility and defect density. Regarding the fill factor (FF) and efficiency, a high defect density or an inappropriate thickness can decrease the FF due to recombination losses, ultimately reducing the overall performance of the solar cell [10].

3.3. Influence of spiro-OMeTAD Layer Doping and Thickness on Electrical Parameters

Figure 4 illustrates the influence of spiro-OMeTAD-based hole transport layer (HTM) doping and thickness on the electrical parameters V_{OC} , J_{SC} , FF, and efficiency in a perovskite solar cell. In this study, doping concentrations were varied from 10^{12} cm^{-3} to 10^{20} cm^{-3} and HTM thickness ranged from 0.02 μm to 0.1 μm . It was observed that all electrical parameters exhibited a similar trend, with improved values as doping concentration and thickness increased. The optimal values were achieved at a doping concentration of 10^{20} cm^{-3} across all electrical parameters. This behavior can be attributed to the effect of HTM doping on hole mobility, which facilitates the transport of holes from the perovskite layer to the cell contacts. Higher doping enhances the electrical conductivity of the HTM layer, thereby reducing voltage losses and improving V_{OC} . However, excessive doping may decrease hole mobility and increase recombination losses, ultimately reducing overall cell efficiency [11]. Similarly, while increasing HTM thickness can initially improve performance, excessively thick layers can result in higher electrical resistance and greater voltage losses, leading to reduced V_{OC} and J_{SC} [12].

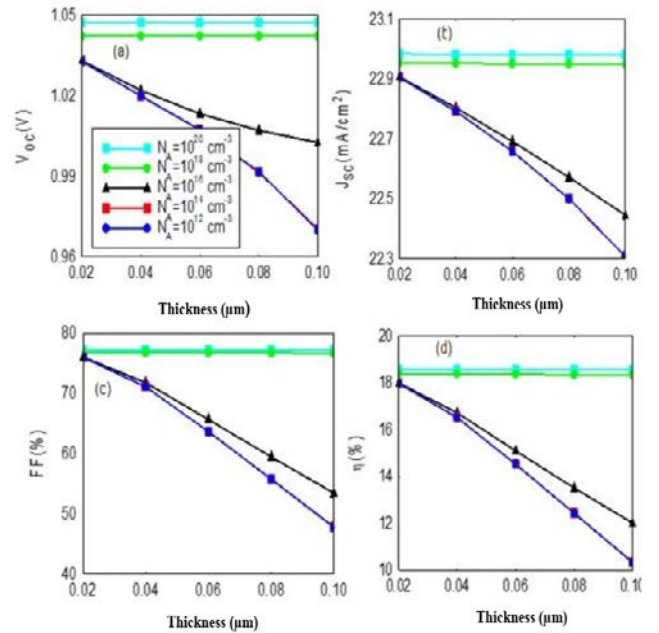


Figure 4. Influence of doping and HTM layer thickness on electrical parameters

3.4. Influence of Mobility and Doping on Electrical Parameters

Figure 5 illustrates the influence of hole mobility and doping levels in the hole transport layer on the performance of perovskite solar cells. It is evident that hole mobility significantly impacts the overall electrical parameters. In Figure 5(a), high V_{OC} values are observed for a doping concentration of 10^{16} cm^{-3} and a mobility of $10^{-3} \text{ cm}^2/\text{Vs}$ [13]. This result arises from the combined optimization of mobility and doping, enabling rapid

charge carrier transport and reducing recombination losses, while optimal doping enhances conductivity and minimizes losses in the HTM layer [14]. In Figures 5(b), 5(c), and 5(d), all parameters progressively increase for mobilities ranging between 10^{-4} and $10^{-3} \text{ cm}^2/\text{Vs}$, all the parameters increase progressively, beyond $10^{-3} \text{ cm}^2/\text{Vs}$, the parameters tend to stabilize. These variations can be attributed to the high hole mobility in the HTM layer, which facilitates efficient charge carrier transport, reduces recombination losses, and improves overall cell efficiency [15]. Furthermore, the doping concentration of the HTM layer plays a crucial role in influencing the electrical parameters such as electrical conductivity. Optimal doping can increase conductivity, which can reduce voltage losses and improve open circuit voltage V_{OC} and current density J_{SC} [16].

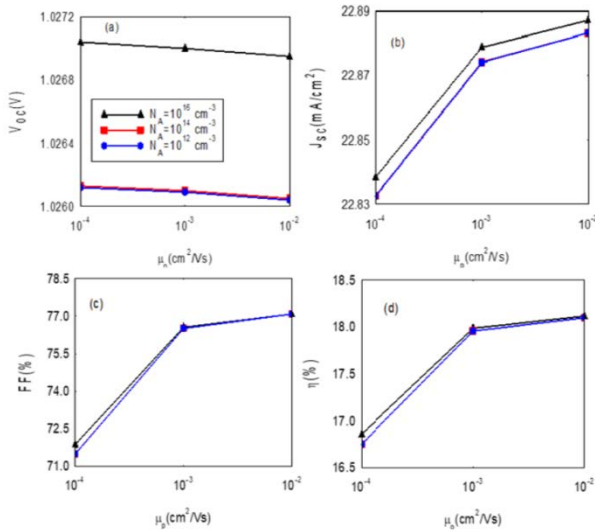


Figure 5. Influence of mobility and doping on electrical parameters

3.5. Influence of Mobility and Thickness on Electrical Parameters

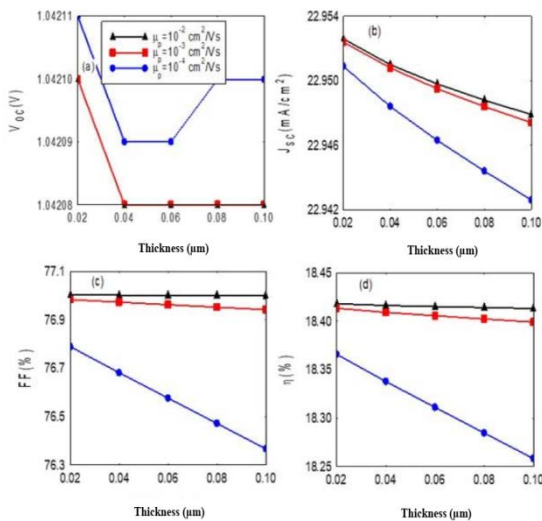


Figure 6. Influence of mobility and thickness on electrical parameters

Figure 6 illustrates the variation in hole mobility as a function of the thickness of the hole transport material layer. It is observed that all electrical parameters decline for a mobility range between 10^{-4} to $10^{-2} \text{ cm}^2/\text{Vs}$, and a

thickness between 0.02 to 0.04 μm . However, a positive trend is noted as the hole mobility increases, as shown in Figures 6(c) and 6(d). This favorable trend could be attributed to improved hole mobility and optimal thickness. Additionally, a mobility of $10^{-4} \text{ cm}^2/\text{Vs}$ appears too low to collect holes, leading to efficient recombination. This explains the decrease in all electrical parameters for low hole mobility in the hole transport material [17].

4. Conclusion

This study investigated the properties of the TiO_2 and spiro-OMeTAD layers on the performance of the perovskite solar cells (PSCs). Through this simulation, we found that for the performance of the solar cells (PSCs), the quality of the TiO_2 and spiro-OMeTAD window layers must be optimal to collect charge carriers at the contacts efficiently. Good performances are observed when the doping of the TiO_2 layer is of the order of 10^{14} cm^{-3} for an ultra-thin thickness and optimum values are obtained for a doping of 10^{20} cm^{-3} and a mobility greater than $10^{-3} \text{ cm}^2/\text{Vs}$ in the spiro-OMeTAD.

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