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RESEARCH ARTICLE

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The role of active and conductive layer thickness in maximizing power conversion efficiency of perovskite solar cells

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Abstract

This study investigates the effect of active and conductive layer thickness on photovoltaic performance in perovskite solar cells, addressing the need for efficient and sustainable energy solutions in light of current environmental challenges. Using OghmaNano software, we analyzed how variations in thickness of the perovskite, fluorine-doped tin oxide (FTO), and gold (Au) layers influence key performance metrics, including power conversion efficiency (PCE), fill factor (FF), open-circuit voltage (Voc), and short-circuit current density (Jsc). The ideal thicknesses identified for achieving maximum PCE are 775 nm for the perovskite layer, 50 nm for the FTO layer, and 100 nm for the Au layer. This study underscores the complex relationship between light absorption and charge transport in perovskite solar cells and highlights the importance of fine-tuning layer thickness for enhanced efficiency. The simulation-based approach used here proves valuable for its practical efficiency, reducing both time and cost compared to experimental fabrication.

Keywords: Perovskite solar cells; layer thickness; OghmaNano software; power conversion efficiency; photovoltaics; sustainable development; nanomaterials

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1. Introduction

Worldwide problems such as rapidly increasing environmental pollution, overuse of natural resources and climate change further emphasize the importance of sustainable solutions in the energy sector as in every field [1]. Renewable energy sources reduce environmental pollution and meet energy needs in a sustainable way. Carbon emissions from the use of fossil fuels have increased the interest in renewable energy sources [2, 3]. Especially solar energy systems minimize the negative impacts on the environment. They also have the potential to generate significant amounts of energy [4, 5, 6]. Recently, technologies such as perovskite solar cells have increased the efficiency of solar energy systems. This has led to significant progress in the field of sustainable energy [7, 8, 9].

Perovskite solar cells have gained an important place in photovoltaic technologies [10]. These cells are in high demand due to their high energy conversion efficiency, low manufacturing costs and flexible design [11]. The rapid advancement of perovskite solar cells in thin film technology allows them to be integrated harmoniously with more flexible and lightweight substrates [12]. This makes perovskite solar cells usable in a wide range of applications, from wearable technologies to sustainable building materials [13, 14]. Perovskite solar cells consist of layers such as FTO, perovskite and metal materials. Each layer is important in determining the overall performance of the solar cell. Therefore, each layer should have an ideal thickness.

OghmaNano software was used in this study. Within the application, the ideal solar cell power conversion efficiency was determined by changing the active and conductive layer thicknesses in the perovskite solar cell structure. Fill factor, open circuit current density and open circuit voltage were also analyzed as efficiency criteria. Perovskite solar cells have high energy conversion efficiency and flexibility of use. They have a significant potential to meet future energy needs [15, 16]. However, in order for this technology to be more widely used in commercial applications, the thickness of each layer needs to be continuously studied and idealized. This study demonstrates the potential to improve the performance of perovskite solar cells. It is also expected to make significant contributions to the future evolution of solar energy technologies.

2. Material and Method

Perovskite solar cells consist of a light-absorbing perovskite layer, electron-hole carrier layers and conductive contacts. TiO_2 is used as the electron carrier layer. Thanks to its high electron mobility and optical transparency, it plays an important role in the charge transport process. Spiro-OMeTAD which is used as a hole carrier layer, supports hole transport thanks to its conductivity which is enhanced by suitable energy levels and doping. The main objective of the study is to determine the ideal thickness of the active and conductive core layers in perovskite solar cells. In this way, the effect of thickness on power conversion efficiency can be understood. These main layers include FTO (fluorine-doped tin oxide), perovskite and Au layers. By varying the thickness of each layer over a certain range, the changes in the performance of the solar cell were investigated. The layer structure of the perovskite solar cell is shown in Figure 1.

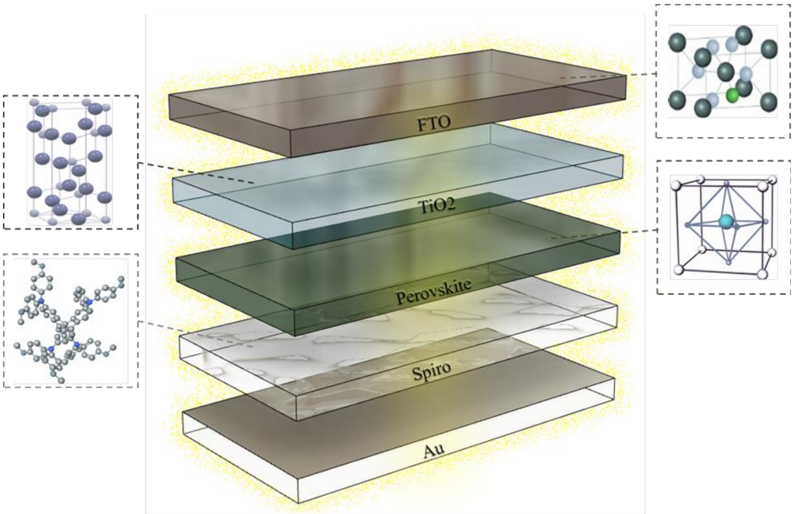

Fig. 1. Layer Structure of Perovskite Solar Cell

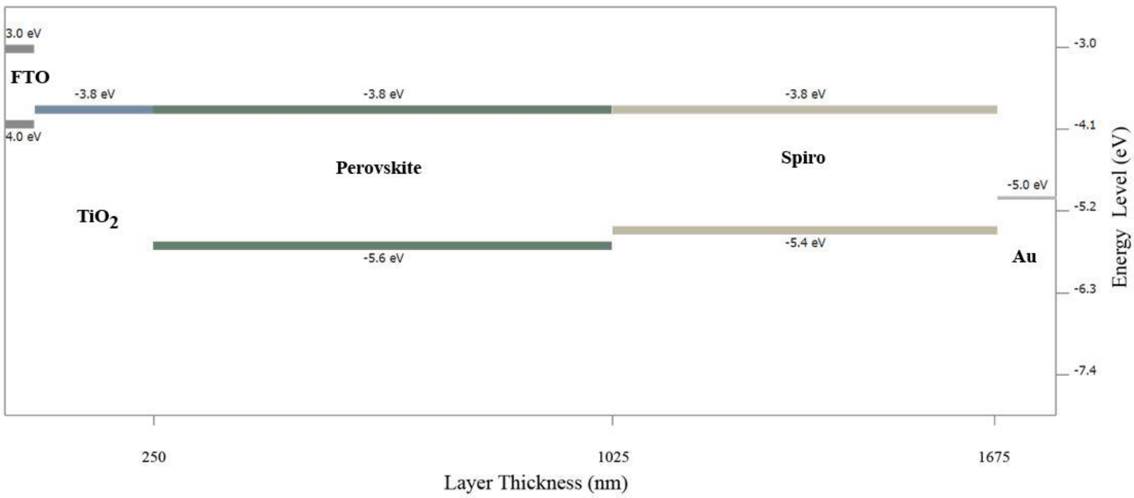

Fig. 2. Energy Levels of Perovskite Solar Cell Layers

Perovskite solar cells consist of basic layers, each playing a different role in the energy conversion process. The perovskite layer absorbs sunlight and generates charge carriers [17, 18]. FTO acts as a transparent conductor. It allows light to reach the perovskite layer [19]. The Au layer acts as an electrode, assisting the electron collection [20, 21]. This strategic combination of layers maximizes light absorption, charge transport and storage, contributing to the overall performance and efficiency of the solar cell.

The layer arrangement and energy levels in perovskite solar cells are shown in Figure 2. The energy levels of the layers created for solar cells vary depending on the operating conditions, the structure of the active layers and the electron carrying capacity. The efficiency of the solar cell should be selected in such a way that these factors will get the best value. There are differences between the energy levels of the cell layers. These differences will allow the electrons excited by the effect of sunlight to create an electric current.

2.1. Perovskite Solar Cell Simulation Indicators

The Fill Factor in the context of a solar cell refers to a critical parameter reflecting the efficiency of the device in converting incident sunlight into electrical energy. It is a quantity that quantifies the extent to which the solar cell operates within the maximum power point of its current-voltage characteristic.

Mathematically, the Fill Factor is defined as the ratio of the maximum power output of the solar cell (P_{max}) to the product of the V_{oc} and J_{sc} [22]. It is shown in the equation (1).

$$Fill\ Factor\ (FF) = \frac{P_{max}}{V_{oc} \cdot J_{sc}} \tag{1}$$

The FF essentially encapsulates losses and deviations from ideality within the solar cell's performance. Factors such as resistive losses, non-ideal diode behavior, and recombination losses contribute to deviations from the ideal behavior. Therefore, a lower FF may indicate inefficiencies or obstructions within the device. A higher FF indicates a more efficient conversion of sunlight into usable electrical power [23, 24, 25].

Power Conversion Efficiency is expressed as a percentage. It is calculated by dividing the electrical power output of the solar cell by the total power of the incident sunlight. The most important factor in determining the efficiency of a solar cell is the PCE percentage, which corresponds to the efficiency of the conversion from sunlight to electrical energy [26, 27]. Mathematically, PCE is given by the equation (2).

$$PCE = \frac{Electrical\ Power\ Output}{Incident\ Solar\ Power}\ x\ 100 \tag{2}$$

The light J-V characteristics were measured under AM 1.5G solar simulator. That is, 1 sun is simulated in AM 1.5G spectrum. P_{in} (1 sun) for AM1.5G is 1000 watts/m^2. Trials were carried out at 300K temperature.

Open-Circuit Voltage (V_{oc}), signifies the maximum voltage the solar cell can achieve in the absence of an external load [28]. Changes in V_{oc} are indicative of the impact of perovskite layer thickness on the cell's ability to maintain a potential difference. V_{oc} is essentially a measure of the potential difference across the solar cell in the absence of current flow, acting as a direct indicator of the built-in electric field within the device [29].

Short-Circuit Current Density (J_{sc}) is denoting the maximum current density attained when the solar cell is short-circuited, effectively acting as a current source [30]. The negative sign of Jsc indicates the direction of current flow. This means that when the cell is short-circuited, current flows through the perovskite layer towards the external circuit. [31, 32].

3. Results and Discussion

3.1. Perovskite Layer

Perovskite solar cells have attracted great interest in the field of photovoltaic technology. The performance of these cells is closely related to the thickness of the perovskite layer [33]. The perovskite layer efficiently absorbs sunlight and produces high-energy electron/hole pairs [34]. In addition, the high conductivity properties of perovskite support the efficient collection and delivery of the produced carriers to the electrodes. Moreover, the layer absorbs a broad spectrum of sunlight by properly aligning the energy levels, improving the overall efficiency of the solar cell [35, 36, 37].

The J-V (current-voltage) graph in perovskite solar cells shows how the solar cell responds to changes in voltage (V) over current (J). This graph is often used to determine the performance of the solar cell. It shows key parameters such as short-circuit current (J_{sc}), open-circuit voltage (V_{oc}) and ultimately maximum power output (P_{max}). J-V curves of perovskite solar cells based on different perovskite layer thicknesses are shown in Figure 3.

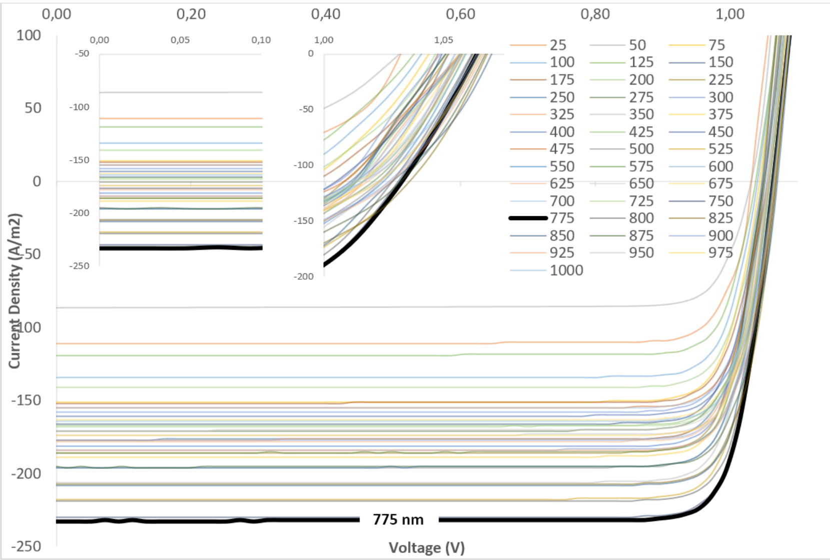

Fig. 3. J-V curves of perovskite solar cells based on different thicknesses of perovskite layers

When Figure 4 is examined, it is seen that the lowest Voc and the highest Jsc occur for the 50 nm thick perovskite layer. This indicates that thinner layers exhibit reduced current generation, which in turn limits light absorption and electron production. On the other hand, the highest Voc and the lowest Jsc values are observed for the 775 nm thick layer. This indicates that thicker layers can contribute to higher voltage and current outputs by increasing light absorption.

The changes in FF, PCE, Voc and Jsc of the perovskite layer are shown one by one in the figure. These parameters show the effect of thickness on the overall performance of the solar cell.

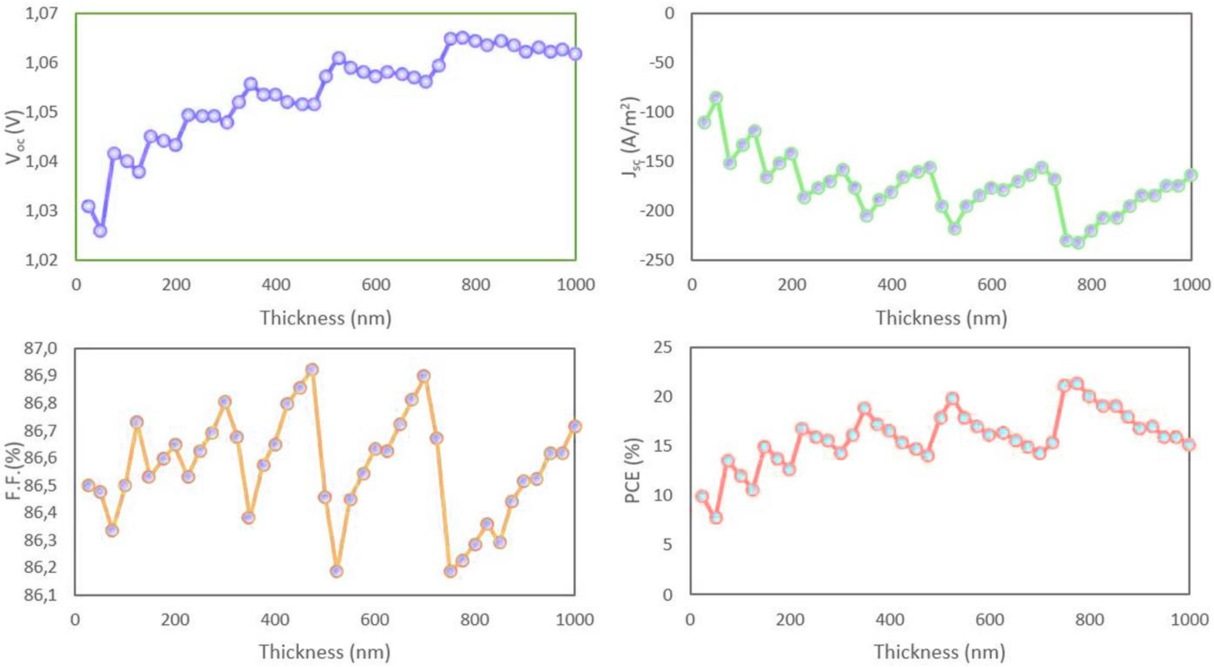

Fig. 4. Effect of change in layer thickness of perovskite on solar cell parameters (Voc, Jsc, F.F. and PCE)

According to the dataset, Voc fluctuates between 1.0259 V and 1.0654 V. Variations in Voc are closely linked to the thickness of the perovskite layer. It affects the cell's ability to maintain the potential difference under the changing layer.

The observed Jsc values range from 232.5062 mA/cm² to 86.3402 mA/cm² is remarkable. It shows the effect of perovskite layer thickness on the current conducting capacity of the cell under short circuit conditions. The fluctuation in Jsc values at different perovskite layer thicknesses shows the importance of the relationship between the optical and electrical properties of the layer.

Fill Factor values range from 0.8619 to 0.8692. These values indicate how effectively the perovskite solar cell uses incoming sunlight to produce electrical power. A higher FF is desirable because it means the solar cell is operating closer to its theoretical maximum power point. This means that overall efficiency is increased.

The observed PCE values range from 7.6594% to 21.3586%. The fluctuations in PCE may be due to various factors related to the perovskite layer. The thickness of the perovskite layer is a factor that determines the optical and electronic properties of the solar cell. When this layer is too thin, there may be insufficient absorption of sunlight. This may result in lower current production. Conversely, an excessively thick layer may lead to increased recombination losses and decreased charge removal efficiency. An ideal thickness is essential to achieve a balance between light absorption, charge carrier production and charge removal. In this study, the perovskite layer with the highest PCE value was measured at 775 nm thickness.

The aim was to evaluate the effects of the perovskite layer on PCE in perovskite solar cells. For this reason, an experimental study was carried out in a wide range between 25 nm and 100 nm by changing the thickness of the perovskite layer every 25 nm. The maximum PCE efficiency in the perovskite layer was determined as 775 nm.

3.2. FTO Layer

In perovskite solar cells, FTO allows light to penetrate the solar cell. It acts as a transparent conductor. It plays an important role in establishing a balance between optical transparency and conductivity. This directly affects the overall efficiency of the solar cell. It also acts as an electrode that actively collects electrons produced during the energy conversion process.

The efficiency parameters for each 25 nm thickness in the FTO layer have been obtained in the range of 25-500 nm. J-V curves of perovskite solar cells based on different FTO layer thicknesses are shown in Figure 5.

Notably, the 50 nm thickness stands out with the highest V_{oc} of 1.0907 V, indicating a potential for elevated open-circuit voltage output. Conversely, the 275 nm thickness demonstrates the lowest V_{oc} at 1.0741 V, suggesting a reduced voltage output. The J_{sc} values follow a similar trend, with the 275 nm thickness displaying the highest current density at 163.9843 mA/cm², for achieving optimal photovoltaic performance. Changes in FF, PCE, V_{oc} and J_{sc} values depending on the FTO layer thickness are shown in Figure 6.

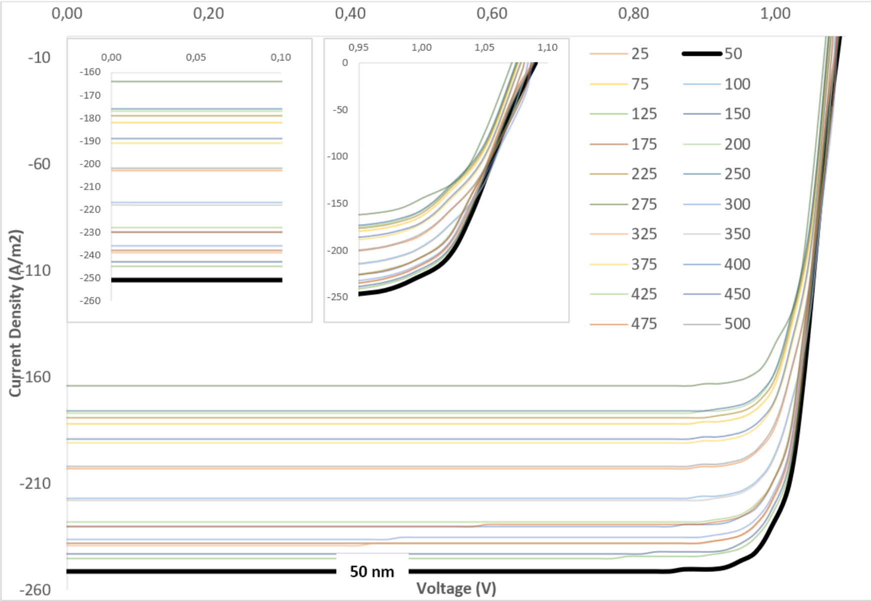

Fig. 5. J-V curves of perovskite solar cells based on different thicknesses of FTO layers

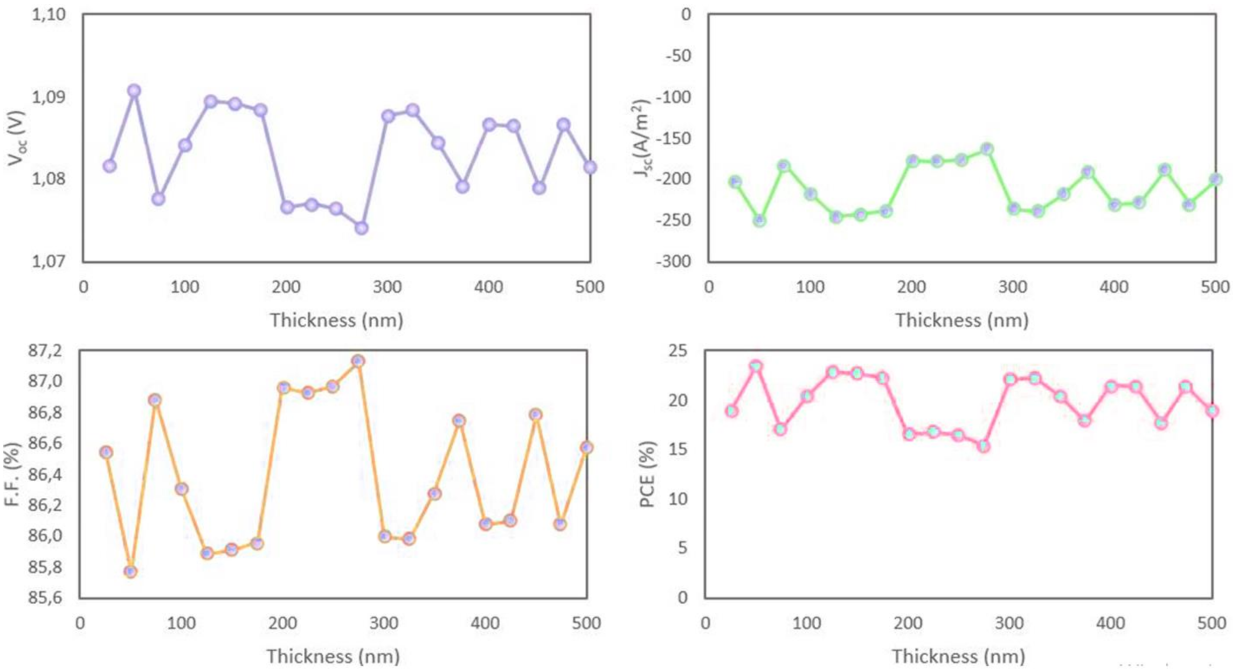

Fig. 6. Effect of change in layer thickness of FTO on solar cell parameters (Voc, Jsc, F.F. and PCE)

As the thickness of the FTO layer increases, the fill factor (FF) exhibits a fluctuating trend ranging between 0.8577 and 0.8713. The power conversion efficiency (PCE) experiences a gradual decrease from 23.4703% to 15.3471%, reflecting the complex interaction between layer thickness and overall cell efficiency. However, these stepwise intervals do not occur in relation to the sequence of thickness values. In other words, as the thickness increases, PCE values have not consistently increased, and occasional declines have occurred. The opposite situations can also occur. As a result, the ideal PCE value of 23.47% was obtained at 50 nm FTO thickness.

3.3. Au Layer

The Au layer in perovskite solar cells serves as an electrode, aiding in the collection of electrons. It plays a crucial role in completing the external circuit and facilitating electron extraction from the solar cell.

The efficiency parameters for each 25 nm thickness in the Au layer have been obtained in the range of 25-250 nm. J-V curves of perovskite solar cells based on different Au layer thicknesses are shown in Figure 7.

The graphical representation of V_{oc} and J_{sc} in relation to the thickness of the Au layer reveals distinctive lines. The 75 nm thick layer stands out with the lowest V_{oc} at 1.0783 V, indicating a notable decrease in voltage output for this particular thickness. In contrast, the 100 nm thick layer exhibits the highest V_{oc} at 1.0907 V, highlighting a positive correlation between increased thickness and elevated voltage. Moreover, the 100 nm thick layer records the lowest J_{sc} at 250.8915 mA/cm². Changes in FF, PCE, V_{oc} and J_{sc} values depending on the Au layer thickness are shown in Figure 8.

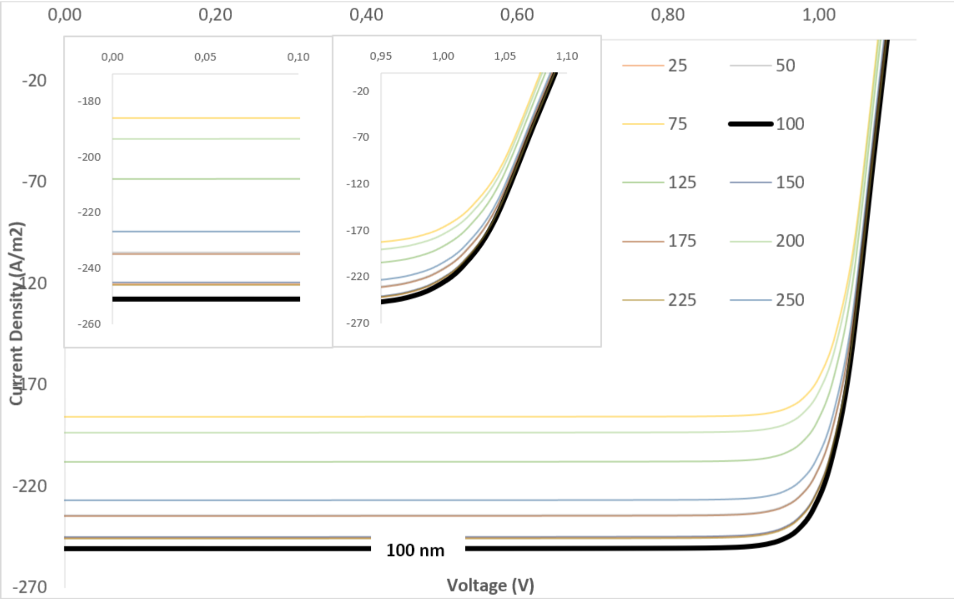

Fig. 7. J-V curves of perovskite solar cells based on different thicknesses of Au layers

The 75 nm thick layer demonstrates the highest FF at 0.8682, indicating an efficient charge transfer and collection for this particular thickness. Conversely, the 25, 100, 150 and 225 nm layer exhibits a slightly lower FF from the 0.8600, suggesting a potential decrease in charge collection efficiency for some other layers. In terms of PCE, the 100 nm thick layer stands out with the highest value at 23.4924%, emphasizing the ideal conversion efficiency achieved at this thickness. The 75 nm thick layer, despite having a high FF, records a lower PCE at 17.4155%, suggesting a potential trade-off between FF and PCE for certain thicknesses.

It is observed that, compared to the maximum PCE values obtained as 17.57% [38], 17,8% [39], 22,06% [40], 19,42% [41], 17,57% [42] and 21,98% [43], the 23.49% PCE value we obtained as a result of the study has a higher value than these studies examined in the literature.

Simulation results show how main performance parameters such as power conversion efficiency, fill factor, open circuit current density and open circuit voltage change depending on the change in the thickness of perovskite, FTO and metal layers. The data obtained emphasize that the optimization of each layer plays a significant role in determining the overall performance of perovskite solar cells.

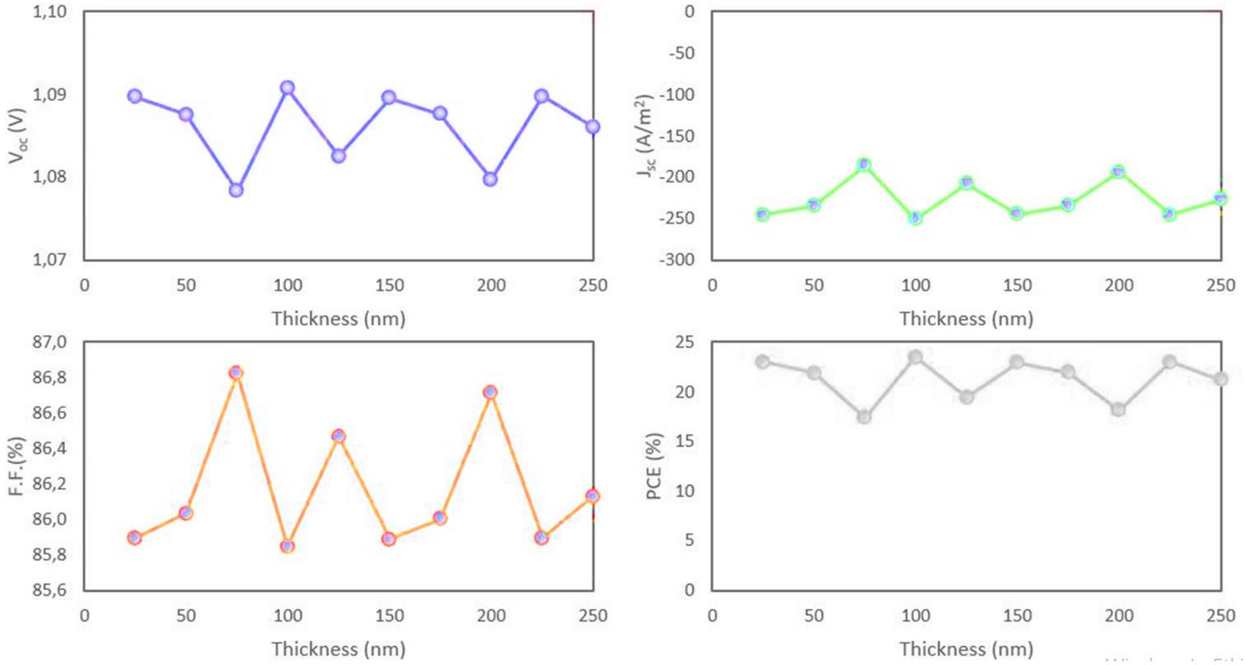

Fig. 8. Effect of change in layer thickness of FTO on solar cell parameters (Voc, Jsc, F.F. and PCE)

4. Conclusion

This study demonstrates that optimization of layer thicknesses in perovskite solar cells can significantly enhance PCE, thus contributing to the development of more sustainable and efficient energy technologies. Using OghmaNano software, we observed that each layer -the perovskite active layer, FTO conductive layer and the Au layer- has an ideal thickness for maximizing the photovoltaic performance of the solar cell.

The highest PCE recorded as 23.49% was obtained from the 775 nm perovskite layer, 50 nm FTO layer and 100 nm Au layers. These thicknesses also produced positive values for other important parameters such as FF, Voc and Jsc. In particular, the optimum 775 nm perovskite layer thickness produced a Voc of 1.0654 V and a Jsc of 86.3402 mA/cm². This indicates that increasing the thickness increases the light absorption and hence produces higher voltage output. However, exceeding this optimum thickness causes recombination losses that reduce the efficiency gains.

The highest PCE value was obtained with the FTO layer thickness of 50 nm. Voc also reached its maximum value at this thickness of 1.0907 V. The results show that thinner FTO layers are generally beneficial for achieving high Voc values due to improved electron mobility. On the other hand, increasing the FTO thickness beyond this value resulted in a decrease in PCE due to excessive material resistance.

The Au layer performed best at 100 nm thickness. It showed a peak Voc of 1.0907 V and a Jsc of 250.8915 mA/cm². At this thickness Au layer collects charges efficiently. Allowing electrons to flow smoothly without adding extra resistance.

This study aimed to find the ideal values of layer thickness in perovskite solar cells to improve PCE, Voc, Jsc, and FF. By fine-tuning these parameters, our findings not only exceed those of previous studies (17.57%, 22.06%, and 21.98%), but also underscore the potential of perovskite solar cells to advance toward practical, high-efficiency applications. This approach to achieving ideal layer properties can serve as a model for future solar cell designs and strengthen the role of photovoltaics in meeting the world's increasing energy demands in a sustainable manner.

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There is no conflict of interest.

Author Contribution

E.N. and M.F.G. organized and performed all the analyses and wrote the manuscript.

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