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Increasing the perovskite cell performance using comparative layering method between PTAA and PEDOT: PSS layers

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ABSTRACT

Today, perovskite solar cells are introduced and used as a suitable alternative with high efficiency for silicon solar cells. The main problem of this type of cells until now has been mostly about their instability, because these materials that are used in perovskite solar cells are rapidly destroyed in reaction with air or their efficiency is greatly reduced. In this article, we increase the productivity to an acceptable amount and also increase its stability by using new high-quality synthesized materials and also by changing the manufacturing method of perovskite solar cells. Using the hole transport layers (HTLs), in the inverse planar perovskite solar cell structure, the effect of two layers of poly (triarylamine) (PTAA) and poly (3,4-ethylenedioxythiophene) (PEDOT): PSS as the bottom layer of the perovskite film on the morphology of the nanoparticles, the crystallinity of the perovskite layer and the photovoltaic parameters affecting the efficiency of the solar cell made in a single-step method were investigated. The result shows the PTAA layer has been very effective in controlling the morphology of the perovskite layer, so the efficiency reached to 23.9% while the maximum efficiency per solar cell based on PEDOT: PSS is 11.37%.

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1. INTRODUCTION

Perovskite solar cells have different layers that the most important of them is perovskite itself, which is very toxic and dangerous. The layers of a cell are arranged in the following order from left to right: Fluorine-doped tin oxide (FTO)/Block TiO_2/Mesoporous TiO_2/Perovskite ($CH_3NH_3PbI_3$)/Spiro-OMeTAD/Au [1], [2]. Figure 1 shows the schematic structure of flat perovskite solar cell.

Substrate preparation: first, it is necessary to etch a surface equal to one third of the substrate to remove the FTO layer from the glass in order to prevent short circuit. For this purpose, zinc powder and two molar hairy cell leukemia (HCL) solutions are used. In such a way that first the powder is poured in a small amount on the desired part and then a drop (depending on the desired surface) of the acid is dripped. After the reaction and the loss of FTO, the cell is washed with deionized water. In order to prevent acid and zinc powder from spreading and corrosion of other parts of FTO, glue can be used. After the etching operation, it is time to wash the substrate or FTOs. Since these cells are highly sensitive to contamination, this step is very important [3], [4]. The washing steps are as follows. FTOs are washed in soapy water and placed in an ultrasonic bath for 10 minutes. Then the same work is done in acetone, ethanol and isopropanol solutions respectively. Of course, the substrates can be washed in hot deionized water between each step. For the final wash, the best option is to use UV-ozone [3], [5].

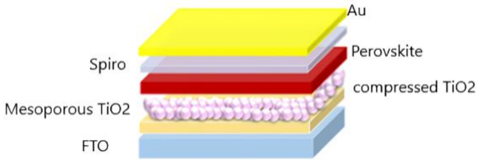


Figure 1. Structure and arrangement of perovskite cell layers

– Compact TiO_2 layer

The compressed layer of titanium oxide is a continuous layer with a maximum thickness of 90 nm, which is coated on all the glass except for the part of the FTO layer that is used as an electrode. Two solutions containing ethanol, transatlantic trade and investment partnership (TTIP) and HCl are combined, passed through a cellulose filter and applied to the glass using a spin coater. After application, this layer is usually dried at 125 °C and annealed at 500 °C for 30 minutes [4], [6].

– TiO_2 mesoporous layer

To prepare the suspension of this layer, titanium dioxide paste and ethanol are used in different proportions. In articles, these two substances are mixed with different ratios of 1 to 6, 1 to 8, 1 to 13, and other ratios. After mixing (using a stirrer), the obtained material is placed in an ultrasonic bath for 2 minutes. Then it can be applied using a rotary layering device. After the address layer, like TiO_2 compressed layer, it is dried at 125° and annealed at 500° for 30 minutes [7], [8].

– Perovskite layer

The most important part in solar cells is the perovskite layering shown in Figure 2. Two methods are often used to make this layer: one-step and two-step perovskite layer fabrication method. Of course, researchers have been able to provide high and acceptable yields by combining these methods with other methods such as Vienna Ab initio Simulation Package (VASP). Here, we explain a two-step method that is very commonly used. Preparation of lead iodide (PbI_2) solution: first, a specific amount of PbI_2 and dimethylformamide (DMF) (as a solvent) are combined to prepare a solution with a specific molarity and placed on a stirrer for 1 hour at a temperature of 80° to 100° until a completely transparent solution is obtained. It is better to carry out all the materials and processes (in order to prevent the entry of moisture and oxygen and as a result reducing the stability of the cells) in the glow box from the PbI_2 production stage. The desired solution is applied to the substrate using a spin coater and annealed at 80° to 120°. Then, to prepare methyl ammonium iodide (MAI) solution, depending on the number of samples, take the required amount of MAI powder (white color) and while it is on the stirrer, add anhydrous isopropanol solvent drop by drop until the desired concentration is reached is added to it. In the following, the immersion method is used for layering this solution.

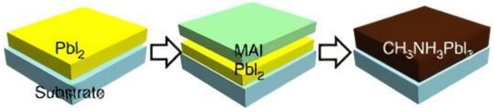


Figure 2. The order of layering steps

In this method, first the substrate is immersed in the prepared MAI solution (until a brown layer is formed on it) and then it is immersed in the isopropanol solution for a few seconds. After that, the sample is quickly placed on the spin coat and dried for about 20 seconds at a specified speed. Then, for the final annealing, it is placed at a temperature of 80°C to 120°C [9]–[12].

– Cavity transport layer

In the construction of this layer, the cells made with spiro-OMeTAD material for the hole transporting layer usually have the highest efficiency. Of course, this material is very expensive and affects the stability of the cell. In this construction method, Spiro’s address layer is explained as a hole transport layer (HTL). In the construction of this layer, the cells made with spiro-OMeTAD material for the hole transporting layer usually have the highest efficiency. Of course, this material is very expensive and affects the stability of the cell. In this construction method, Spiro’s address layer is explained as a HTL. After making both solutions, a certain amount of the second solution is added to the first solution, and then the final solution is placed on the stirrer for 30 minutes at a temperature of 60 °C while stirring. After this step, the solution is filtered by a filter with a size of 0.45 μm. To apply the layer, a certain amount of the solution is poured on the sample (FTO/Block TiO_2/Mesoporous TiO_2/Perovskite) and the address layer is done by the spin coating machine [13]–[15].

– Gold electrode deposition

In this stage, which is one of the most important stages of layering, two materials, gold and silver, are used. Each of these materials has its own properties, quality, and productivity. Gold is excellent because of its high efficiency, but maybe because of its high cost. It is little used. We are dealing with gold plating here. The gold layer is a very suitable option in this type of solar cells due to its work function and energy level of 1.5 eV (next to the Spiro layer with an energy level of 2.5 eV). This layer is layered by thermal evaporation layering method. The desktop sputtering device is used in specialized laboratories to facilitate the process of sample preparation before performing the field emission scanning electron microscopy (FESEM) test. With the addition of this gold coating device, FESEM imaging will be done faster. This device is capable of coating targets made of noble metals such as gold, platinum and palladium, silver, aluminum by sputtering method and is mainly used as a cover for electron microscope samples in research laboratories. Also, this device with the ability to be equipped with a carbon system of carbon thread also provides thermal evaporation. Process with automatic or manual control of the vacuuming and layering process, layers with a thickness of 1 nanometer can be produced [16]–[19].

2. PROBLEM SOLVING

The materials used in the different layers of a perovskite solar cell are always one of the most important challenges for researchers in the layering of those layers. For example, some materials do not spread evenly when layered with a spin coater, so we propose the high-quality synthesized materials in this research and compare them with each other. Excellent chemical compounds such as carbon-containing compounds are one of the solutions proposed in this field. Also, by changing the thickness of the layers, you can see the difference in the efficiency of these cells. Considering that perovskite solar cells are under the nano branch, if it is possible to find to reduce the thickness of HTL and electron transport layer (ETL), it can be hoped that in the future, using nano technology and semiconductors, smaller and lighter solar cells more and also with the highest production efficiency. In this research, in the laboratory environment and by using the synthesis of organic materials, as well as the changes that can be made in different layers of a cell, to check how much the stability and productivity of the perovskite cell will change. It has also checked how long the current voltage drop occurs. Other important factors investigated in this research are: the amount of sunlight, the thickness of the layers, the type of coating, the process of making the base cell, and the amount of organic materials used [20]–[23].

2.1. The process of making and applying changes

In this research, from the structure of inverted planar perovskite solar cell due to its prominent features, including the construction in low temperature and low manufacturing cost have been used. Perovskite layer morphology and parameters affecting the performance of solar cells were investigated and atomic force microscopy (AFM) images showed the appropriate morphology and high coverage of the perovskite film on poly (3,4-ethylenedioxythiophene) (PEDOT) doped with poly (styrene sulfonate) (PSS) anions compared to the film on poly (triarylamine) (PTAA) [24]–[29].

2.2. Materials and equipment used

Solvents: acetone, ethanol 98%, toluene 98%, N,N-DMF, and dimethyl sulfoxide (DMSO) from the company Merck, lead iodide (2) PbI 99%, MAI 98%, PTAA and PEDOT: PSS from Sigma-Aldrich, (6,6)-Phenyl C61 butyric acid methyl ester (PCBM), and Bathocuproine (BCP) prepared by Ossila company [30], [31].

3. RESULTS AND DISCUSSION

3.1. Construction method

Indium tin oxide (ITO) is used as a substrate to make perovskite solar cells. Figure 3 shows the schematic structure of perovskite inverted planar solar cell. Thin film and nanostructured solar cells are very sensitive to contamination of the substrate surface, so the substrates are washed in several steps. The ITOs are washed with soap and water and placed in an insulated container, they are rinsed with a solution of doubly distilled (DI) water, acetone, and ethanol. Each of them is placed in an ultrasonic bath for 15 minutes. Then the substrates are dried with N_2 gas flow to complete the washing step. Next, for the HTL layer, the hole transporter, first the amount of 2.5 mg of PTAA and dissolved in 1 ml of toluene, then PTAA and PEDOT: PSS solution using a spin coater machine with two speeds of 5000 rpm and 6000 rpm and for 60 seconds. The order is added to the upper layers and the ITO layer at high temperature. They are dried at 110 and 150 °C. To form the perovskite film by one-step method of PTAA and PEDOT: PSS layers, perovskite solution consisting of 461 mg of lead iodide, 159 mg of magnesium powder, 635 μl of MFD and 71 μl of DMSO using the spin-coater method on the HTL substrate it will be added. Then, ETL and HTL are layered with PCMB and BCP at 6000 and 9000 speeds respectively on the spin coater in two separate steps. Finally, a thin layer of aluminum with a thickness of 50 nm is placed on the BCP layer by vacuum evaporation method [32]–[34].

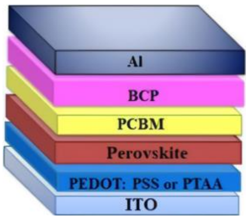


Figure 3. Inverse planar perovskite solar cell structure

Figures 4(a)-(d) shows the structure of PTAA, PEDOT: PSS, PCBM, and BCP molecules. In addition to being a suitable electron carrier, PCBM material can increase performance and reduce waste in solar cells and can be converted to perovskite. BCP material is useful as a hole barrier, in addition, it can prevent hole passage like a barrier due to improved electron transport.

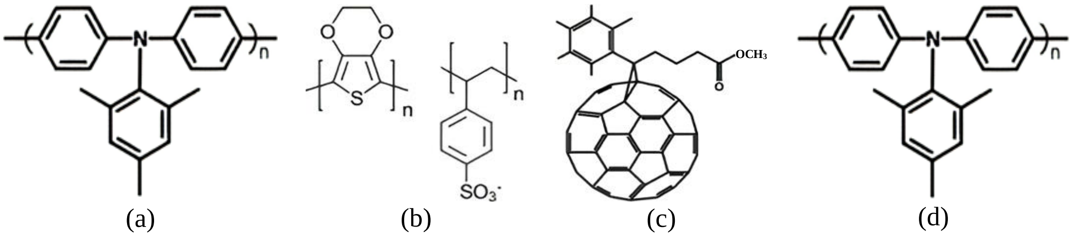


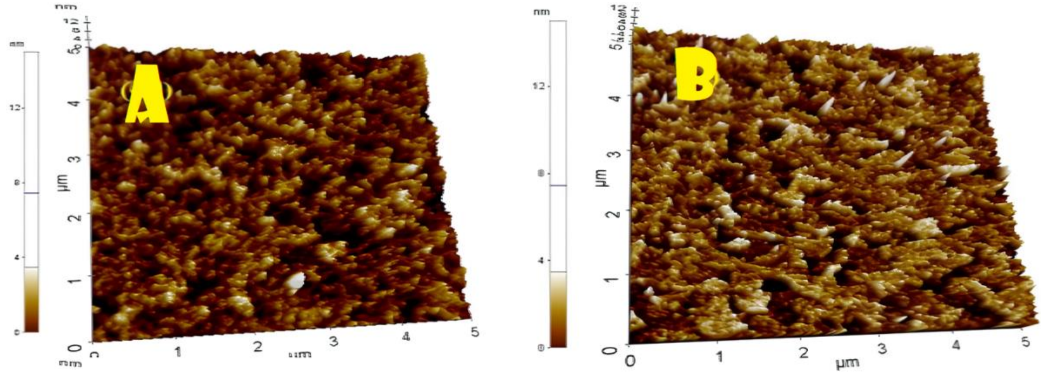
Figure 4. Molecular illustration of: (a) PTAA, (b) PEDOT: PSS, (c) PCBM, and (d) BCP structures

PEDOT: PSS and PTAA materials are used for HTL layers. They fit the holes and are considered as the substrate of the perovskite film, as can be seen from the diagram in Figure 4. Therefore, having a suitable coating of these materials increases the quality of the perovskite film. Another parameter affecting the performance of crystalline perovskite solar cells and the morphology of nanoparticles is the perovskite layer.

Figure 5 shows the atomic force microscopy (AFM) image of the surface of the perovskite film on PEDOT: PSS and PTAA hole transport materials. The small holes on the surface of the perovskite film coated on PEDOT: PSS surface as shown in Figure 5(a), indicate the destruction of the PSS chain in the PEDOT: PSS film. It seems that the DMSO solvent in the perovskite solution in the process of layering and preparing the perovskite film caused the destruction of the PEDOT: PSS film. The size of small perovskite crystals increases the number of grain boundaries and is also a destructive factor in device performance. It has been found that the presence of small holes and the increase in the number of grain boundaries in the perovskite layer increases the recombination of electrons and ultimately limits the stability and performance of the device [35]–[38].

The dark spots in the AFM image of the perovskite film coated on the PTAA surface in Figure 5(b) shows the morphology of nanoparticles in the perovskite layer grown on PTAA substrate have a denser coverage. By covering with a layer of nanoparticles, the perovskite layer increases light absorption and solar cell efficiency.

It may decrease the open circuit voltage and destroy the efficiency of the solar cell. The graph of the absorption spectrum for both cells made with PSS hole transporters: PEDOT and PTAA can be seen in Figure 6. The presence of holes and the very small size of nanoparticles of the perovskite film based on PEDOT: PSS, which increases the grain boundaries also cause a decrease in absorption in this perovskite film compared to PTAA-based perovskite (absorption diagram in Figure (6). It can be seen that the presence of a small amount of PbI_2 in the perovskite film is confirmed which is useful for achieving higher open-circuit voltage [39]–[41].



(a) (b)

Figure 5. AFM images of perovskite cells fabricated on transfer layers PSS hole donor: (a) PEDOT and (b) PTAA

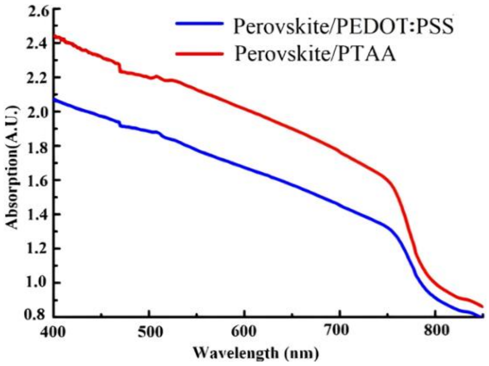


Figure 6. Absorption spectrum diagram made of perovskite cells, overlays PSS hole transporter: PEDOT and PTAA

Investigating the effect of the thickness of PEDOT: PSS and PTAA hole carrier layers on solar cell performance and photovoltaic parameters, short circuit current density (J_{SC}), open circuit voltage (V_{OC}), fill factor (FF), and power conversion efficiency (PCE), using a 2400 Keithley device and solar simulator was converted by mining 5G.1 AM. It should be noted that the power conversion efficiency of the solar cell depends on three photovoltaic parameters (FF, V_{OC}, and J_{SC}). The (1) and (2) show the dependence of power conversion efficiency on these parameters. In these relationships, V_{max} and J_{max} are the maximum voltage and maximum current density, respectively. P_{in} is the power of light [42]–[44].

$$FF = \frac{V_{max} \times J_{max}}{V_{OC} \times J_{SC}} \tag{1}$$

$$PCE = \frac{V_{OC} \times J_{SC} \times FF}{P_{in}} \tag{2}$$

The results of photovoltaic parameters and their values are given in Table 1.

Table 1. Table of photovoltaic parameters

Cavity transporter	J_{SC} (MA/cm^2)	FF%	VOC(v)	PCE%
PTAA	17.25	68.8	1.07	23.9
PEDOT: PSS	12.97	64.2	1.03	11.37

As can be seen from the results in the table, the efficiency of perovskite solar cell made based on PTAA is 23.9%, while the efficiency of perovskite solar cell with PEDOT: PSS layer is 11.37%. This increase in efficiency is because the current density and fill factor in the case of PTAA are higher than the cell based on PEDOT: PSS. The reason for the improvement of FF is the morphology of the nanoparticles and the quality of the layers, especially the perovskite layer. In fact, the PTAA layer improves the quality of the perovskite layer and creates a denser perovskite coating, the number of holes in this perovskite film is less, and these factors improve the FF. On the other hand, the high quality of perovskite layers is another reason for more electron-hole transfer and improved mobility of charge carriers, which improves J_{SC}. One of the factors influencing the increase of Voc in perovskite solar cells is the selection of hole filling materials with suitable energy band gap. The improvement of Voc in the solar cell with PTAA HTL is due to the relatively large energy band gap of this material. The current-voltage density diagram of cells with PTAA and PEDOT: PSS transporter and the schematic structure of the solar cell band gap are shown in Figures 7 and 8, respectively [45]–[48].

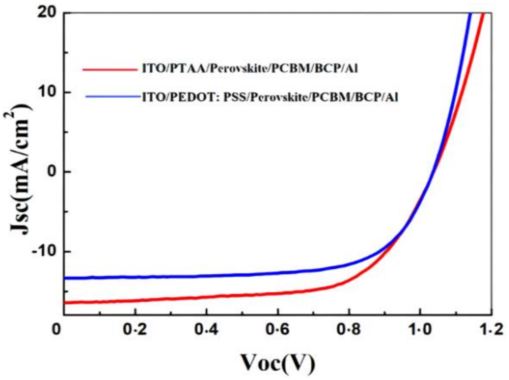


Figure 7. Current-voltage density diagram for perovskite solar cell with PTAA and PEDOT: PSS HTLs

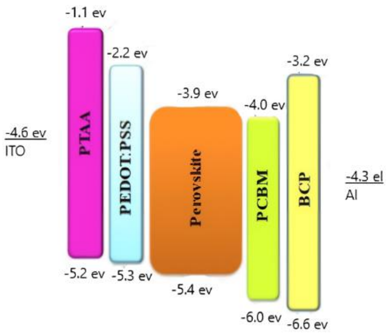


Figure 8. Schematic of voltage band gap structure for solar cell perovskite

According to Figure 7, it can be seen that in two perovskite solar cell manufacturing modes, the method in which PTAA is used has a higher efficiency than the PEDOT: PSS method, and the blue graph shows it. In Figure 8, we see a comparison of the types of electron absorption layers, which shows the maximum and minimum layers. According to the type of application for which the layers are used, the desired layer can be selected in the active layer [47]–[50].

4. CONCLUSION

In this research, using HTLs, in the inverse planar perovskite solar cell structure, the effect of two layers of PTAA and PEDOT: PSS as the bottom layer of the perovskite film on the morphology of the nanoparticles, the crystallization of the perovskite layer and the photovoltaic parameters affecting the efficiency of the solar cell made in a single-step method were investigated. The size of perovskite nanoparticles formed on the PEDOT: PSS surface is smaller than that of PTAA, therefore, the number of grain boundaries in the PEDOT: PSS perovskite layer is higher and also the morphology of the PTAA-based perovskite layer has better quality and compactness, while there are micro-holes in the morphology of perovskite coated on PEDOT: PSS. Because of the state of DMSO in the perovskite solution, in the process of coating and preparing the perovskite film, the PEDOT: PSS film has been destroyed and created holes in the perovskite layer. Therefore, the improper morphology of the PEDOT: PSS-based perovskite layer increases the electron-hole recombination and reduces the performance of the solar cell. As a result, the PTAA layer has been very effective in controlling the morphology of the perovskite layer, so the efficiency reached 23.9% while the maximum efficiency of solar cell based on PEDOT: PSS is 11.37%.

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