An Overview of the Inverted Polymer Solar Cell Architecture's Development

Mr. Rajkishor Singh, Mr. Shoyab Hussain, Mr. Jitendra Kumar Singh Jadon

[1,2,,3]Shobhit Institute of Engineering and Technology (Deemed to be University), Meerut

Email id- rajkishore@shobhituniversity.ac.in, shoyab.hussain@shobhituniversity.ac.in, jitendra@shobhituniversity.ac.in

ABSTRACT: The rising cost of producing energy from fossil fuels has prompted a quest for a more cost-effective alternative energy source. Solar energy is one alternative energy source that has piqued my attention. Organic semiconductor polymer solar cells are a potential alternative to inorganic materials because they are cheaper, lighter, more flexible, and can be manufactured into huge regions using roll-to-roll manufacturing. The traditional design for manufacturing solar cells, on the other hand, requires a high vacuum to deposit the top metal electrode, which is not appropriate for roll-to-roll production. Recently, an inverted device design was explored as a possible architecture for creating optimal roll-to-roll polymer-based solar cell manufacturing. The latest developments and methods in the creation of this kind of inverted device design will be discussed in this study. We'll go through some of the work we've done to combine the inverted device architecture platform's materials, device, interface, and manufacturing to create more idealized polymer-based solar cells.

KEYWORDS: Interface Engineering, Inverted Device Architecture, Polymer Solar Cell, Self Assembled Monolayers, Solar Cell

INTRODUCTION

Organic polymer photovoltaic cells have recently received a lot of attention as a result of the need to create a low-cost, clean, and long-lasting renewable energy source. Polymer-based solar cells having the benefit of being less costly and solution process able using roll-to-roll methods[1]. A solution processed p-type poly(3-hexyl-thiophene) (P3HT) polymer and an n-type -phenyl C61 butyric acid methyl ester (PCBM) fullerene make up the most extensively investigated polymer blend system. This polymer mix method has resulted in efficiencies of up to 5%. 2,3 By creating smaller band-gap polymer materials that can absorb a wider range of the solar spectrum, polymer: fullerene bulk-heterojunction (BHJ) systems with efficiencies as high as 6 to 7% have been obtained[2]. The BHJ device design is accomplished by combining n-type and p-type materials to increase the number of interfaces between the donor and acceptor phases, allowing for more exciting dissociation/charge separation sites and therefore more charge carriers to be generated. Owing to the poor mobility of the conjugated materials, higher phase segregation of the mix materials will result in reduced photocurrents due to increased charge recombination rates. The BHJ idea has been included into most traditional device architectures[3].

A transparent conducting metal oxide is covered with a poly hole-transporting layer, which is followed by the active BHJ layer in this design. As an electron-collecting electrode, a low work function metal electrode is evaporated on top to complete the device. Although the majority of polymer-based solar cells are manufactured using traditional methods, there are issues about device stability[4]. When exposed to the acidic PEDOT: PSS hole-transporting buffer layer, the transparent conducting indium tin oxide (ITO) employed as the hole collecting contact may be etched over time. Due to the high resistance of the transporting layer, replacing the PEDOT: PSS layer with alternative hole-transporting layers has so far failed to maintain high conversion efficiencies. Because of the low work function electrode employed in this device design, high vacuum deposition is required, resulting in higher manufacturing costs[5]. Furthermore,

exposure to the environment may cause oxidation of these electrodes, resulting in device deterioration and failure. Between the top metal electrode and the organic active layer, electron selective buffer layers (TiO2, ZnO) have been effectively placed to reduce oxygen diffusion and enhance device stability. To finish the device, however, high vacuum deposition of metal electrodes is still required. Device designs that do away with PEDOT: PSS at the ITO interface and replace it with non-vacuum deposited high work function metal electrodes at the top interface are required. Based on these concerns, an inverted device design was suggested as a viable device alternative, with the mechanism of charge collection reversed. Due to the device stability and processing benefits of this design over traditional architecture, it has lately attracted a lot of research interest[6].

The polarity of charge collection is reversed in this inverted design, enabling greater work function (Au, Ag, Cu) and less air-sensitive electrodes to be used as the top electrode for hole collection. Higher work function metals provide improved ambient interface device stability and the ability to deposit the top electrode using non-vacuum coating methods, reducing fabrication complexity and costs. The majority of the research focus on these inverted device designs has been on figuring out how to enhance the device's efficiency, stability, and processing of the many interface levels[7]. The orientation of the incoming light source lighting the solar cells top lit or bottom illuminated solar cell architecture distinguishes the inverted design. The bottom illuminated inverted architecture configuration uses a higher work function reflective electrode as the top hole collecting contact and a semi-transparent conducting electrode at the bottom to collect electrons, whereas the top illuminated architecture uses a reflective buried bottom electrode and a semi-transparent top electrode. Although both of these inverted solar cell designs have been successfully shown in the literature, the majority of study has concentrated on the bottom illuminated type inverted solar cell. This is owing to the difficulties of obtaining a clear conducting top electrode material that is appropriate for top lit devices[8].

The top electrode must be semi-transparent in order for light to reach the active layer in the top lit inverted solar cell design. A thin layer of aluminum was placed over glass, followed by a titanium film, in this kind of building. On top of it, a polymer active layer was applied, followed by a PEDOT: PSS Au grid layer. The PEDOT: PSS grid semi-transparent top electrode arrangement showed 1.4 percent efficiency. Chen et al. also developed a 3 percent efficient top lit type inverted device. The distinction in this device design was that instead of a glass substrate, a flexible stainless steel metal foil was utilized as the substrate. Ag, ITO, Cs2CO3, P3HT: PCBM active layer, MoO3, Al metal grid, and ITO were the layers placed on top of the stainless steel foil in that order. Due to the fact that these devices were manufactured on flexible foils, a flexural test was conducted, which revealed excellent mechanical stability and only a 12% reduction in efficiency after 450 bending cycles[9]. On a polymer flexible substrate, the top illuminated inverted arrangement was also demonstrated. A surface-nickelized polyimide sheet was utilized instead of a metal foil. On the surface nickel zed polyimide film, a thin layer of titanium oxide precursor was cast, followed by a P3HT: PCBM active layer and a high conductivity PEDOT: PSS top electrode with a 2.4 percent efficiency[10].

DISCUSSION

A high work function electrode is employed at the top to collect holes in the bottom lit inverted solar cell arrangement, and an interface layer is used to alter the ITO interface to efficiently collect electrons. Cs2CO3,20,21 Ca,22 ZnO,10,23,24 and TiO2 are some of the interface layers that have been used to alter ITO for efficient electron collecting. The layers are usually

extremely thin to ensure high transparency since light must flow through them to reach the active layer to create a photocurrent. Because direct contact between the top high work function metal and the active layer may degrade solar cell efficiency, hole transporting electron blocking films have been placed between these layers to enhance charge selectivity and hole collecting. Various transition metal oxides have been used at the active layer and metal contact in certain materials. Because of their high optical transparency in the visible and near infrared, high carrier mobility, and solution processibility, N-type metal oxides (ZnO and TiO2) are more frequently used as the interface modification layer at the ITO interface for inverted solar cells. These metal oxides' energy levels (LUMO and HOMO) have been calculated to be approximately 4.4 and 7.6 eV, respectively.

These materials are excellent electron selective layers and hole-blocking layers because to their low LUMO and high HOMO values. The use of these n-type metal oxide layers as the electron selective layer for inverted solar cells has been shown many times in the literature. An effective inverted solar cell using a high temperature processed sol-gel ZnO under layer on ITO and an Ag electrode as the top hole collecting contact. Thermal annealing of the ZnO sol-gel at 300°C for 5 minutes improved its conductivity and mobility, resulting in conversion efficiencies of 2.97 percent. It was discovered that when these gadgets were exposed to air, their performance increased. They credit the improvement to Ag oxidation, which caused the effective work function to move closer to the HOMO of P3HT, resulting in better ohmic contact. Even after 7 days of storage, devices kept in nitrogen with occasional exposure to air maintained a device efficiency of 2.32 percent. At the ITO interface, a thin titanium oxide sol-gel layer (10 nm) was also shown to be an efficient electron selective layer for usage in inverted solar cells.

Devices were made using a P3HT: PCBM solution in o-xylene with a solution processed PEDOT: PSS interface layer between the active layer and the Au top electrode, with efficiencies of 3.1%. The scientists discovered that employing o-xylene as a solvent segregate more PCBM at the bottom electron collecting interface, making inverted solar cells more efficient. To reduce losses in photocurrent and efficiency induced by charge recombination owing to poorly distributed phases, controlling the bulk blend vertical phase segregation of one of the materials towards a certain charge collecting interface is critical. Many research groups have previously shown that vertical phase segregation of the donor and acceptor mix materials in the bulk-heterojunction has a significant impact on the performance of polymer-based solar cells. In another research, the same group covered the ITO surface with a thin polyoxyethylene tridecylether (PTE) layer (10 nm) before depositing a thin titanium oxide layer in an inverted solar cell, resulting in efficiencies of 3.6 percent.

The passive PTE layer is thought to enhance the surface quality for improved titanium oxide wetting of the surface, resulting in a more intimate contact with the active layer. Inverted polymer-based solar cells provide good thermal stability. Another issue with polymer-based solar cells is the morphological stability of the BHJ blend phases, in addition to ambient device stability. Because the materials still have a degree of flexibility to diffuse slowly or recrystallize over time, the phase-separated morphology of the blends is not particularly thermodynamically stable. This is particularly true at high temperatures, when progressive changes in nanostructure and microstructure may occur. The two components will separate into bigger phases, resulting in a decrease in the number of interfaces and a decrease in device performance. To enhance the thermal and morphological stability of P3HT: PCBM BHJ active layers, various methods have been explored. The first is to alter the polythiophene backbone in order to introduce a regulated degree of disorder, which aids in suppressing crystallization-driven phase separation between the polymer and fullerene. Another option is to use diblock copolymer additives in the BHJ

film to assist stabilize the film and prevent phase separation. Another technique for stabilizing Nano phase segregation that has been shown to be successful is to employ comparable chemical motifs in both the polymer and fullerene utilized in the blend system. Amorphous fullerene derivatives are produced and used as the electron accepting material in BHJ inverted solar cells based on P3HT: fullerene. The amorphous fullerenes investigated are made by substituting the planar phenylene ring with a bulky diphenylamine in PCBM. Despite the fact that acceptable efficiencies have been achieved using n-type metal oxides as the electron selective layer in inverted solar, it is well known that metal oxides contain hydroxyl groups on their surfaces, which have been proven to induce charge trapping at the interface. 54 Due to poor charge transfer, these hydroxyls terminated surfaces cause significant charge carrier recombination, resulting in device performance losses. To enable effective charge collection, this increase in resistance across these interfaces must be reduced by properly regulating the electrical contacts contact resistance, charge transfer, and energy level alignment.

Furthermore, owing to significant recombination of charge carriers, a poor morphological distribution of phases in the bulk-heterojunction active layer may result in high resistances in the solar cell. The size and distribution of phases must be properly regulated to enhance device characteristics and reduce resistance losses in the active layer. A self-assembled monolayer (SAM) between the inorganic and organic interface may decrease resistance across the metal oxide interface while also affecting the active layer shape. SAMs may be used to substantially alter the interfaces between oxide and metallic surfaces in order to enhance adhesion, compatibility, charge transfer characteristics, energy level alignment, and material development. We've shown that using a fullerene-based self-assembled monolayer (C60-SAM) to alter the metal oxide surfaces of TiO2 and ZnO-based inverted solar cells may enhance device performance. The C60-SAM influences photo induced charge transfer at the interface, reducing charge recombination, passivating inorganic surface trap states, improving exaction dissociation efficiency at the polymer/metal oxide interface, and acting as a template to influence the over layer bulk-heterojunction distribution of phases and crystallinity, resulting in higher efficiency inverted solar cells. The active layer film manufacturing conditions may have a significant impact on the final device efficiency.

 The mix ratio of donor and acceptor materials, the active layer film thickness, the thermal annealing temperature, and the thermal annealing duration are all processing parameters that may influence device efficiency. Using a P3HT: PCBM blend ratio of 1:0.7, an active layer thickness of 200 nm, and an annealing temperature and duration of 160°C for 10 minutes, the optimal active layer efficiency in C60-SAM modified inverted solar cells is determined to be 4.5 percent. The efficiency improves from 1.0 percent to 2.7 percent in unmodified devices and from 1.6 percent to 3.5 percent in C60-SAM modified devices when the ratio is increased from 1:0.3 to 1:0.4. The fill factor and of the unmodified devices are still low (47.6% and 9.0 mA/cm2, respectively), suggesting resistances in the solar cell, but following modification with a C60-SAM, the fill factor and are increased to 52.2 percent and 10.3 mA/cm2, showing resistances in the solar cell. This demonstrates that the SAM has an effect on the mix active layer shape, lowering resistance losses due to carrier recombination. Both the changed and unmodified devices exhibit saturation in the device when the mix ratio is increased from 1:0.5 to 1:1. When compared to devices without modification, the C60-SAM devices exhibit improvements in and FF at greater mix ratios. At 1:0.7 mix ratios, the greatest PCE was 4.5 percent. The C60-SAM impact on bulk morphology to enhance solar cell efficiency is minimal at these ratios. As a result, at these larger ratios, the improvement from the C60-SAM is mostly attributable to better charge transfer characteristics at the interface. The Effect of BHJ Film Thickness on the Performance of Inverted Solar Cells. The BHJ layer thickness is another

factor that may affect the inverted solar cell's performance. Inverted solar cells were spun at 1500 rpm with solution concentrations ranging from 10 mg/mL to 60 mg/mL, and the impact on the four device characteristics.

The BHJ film thickness in these inverted solar cells was optimized using a mix ratio of 1:0.7 and an annealing temperature of 160°C for 10 minutes. With a 10 mg/mL concentration, the Voc is low (0.53), but when the solution concentration rises film thickness rises, the Voc rises and stays comparable (0.61–0.63 V). The lower Voc in the thin layer may be due to the development of additional current leakage channels in the film, resulting in more charge recombination. The rises as the BHJ film thickness increases owing to the film's greater optical absorbance, which generates more charge carriers. The FF is low with a thin BHJ film (10 mg/mL), but increasing the film thickness results in fill factors higher than 60%. However, increasing the thickness reduces the fill factor owing to the active layer's high resistance caused by the organic materials' poor charge carrier conveyance. The optimal BHJ film thickness would optimize photon absorption while maintaining high carrier mobility to allow for maximal charge collection. In these inverted solar cells, the BHJ film thickness of 200 nm (40 mg/mL) is shown to have the best PCE. The Effect of Thermal Annealing Temperature on Inverted Solar Cell Performance. The thermal annealing of the BHJ mix is another manufacturing parameter that may affect solar cell performance. Annealing may affect the number of interfaces for exciton dissociation by changing the mix shape and segregation of donor/acceptor phases. The device performance of inverted solar cells with thermal annealing temperatures ranging from 100 to 200 degrees Celsius was investigated using a BHJ film thickness of 200 nm, a blend ratio of 1:0.7, and an annealing duration of 10 minutes. The annealing temperature had a little impact on Voc until it reached 200°C, when it dropped to 0.57 V. In devices with annealing temperatures ranging from 130°C to 160°C, the highest is observed. This is further reduced when the annealing temperature is raised. The FF, on the other hand, exhibits a significant variation in annealing temperature. Temperatures below 120°C result in fill factors of less than 50%. Fill factors as high as 65 percent are achieved by raising the temperature from 130°C to 170°C. Increased temperatures over 170°C, on the other hand, result in a lower fill factor. The development of the blend morphology, as defined by AFM, explains this dramatic shift in the fill factor.

Low annealing temperatures do not enable the P3HT and PCBM to interact significantly, resulting in limited mobility in the organic material phases and excessive carrier recombination. The thermal energy needed for both the P3HT and PCBM to pack and interact at high temperatures (130°C to 160°C) is adequate to enable the phases to segregate into the optimal Nano phase shape. The size of the phases begins to increase at higher temperatures (170°C to 200°C), as seen by the AFM pictures. The number of surfaces for exciton dissociation is reduced in these bigger phases, resulting in greater charge carrier recombination and a decrease and FF. The ideal annealing temperature for obtaining the PCE is 160°C. The Effect of Thermal Annealing Time on Inverted Solar Cell Performance. The Effect of the Top Metal Anode Electrode on Inverted Polymer Solar Cell Performance. The type of charge collection at the active layer/electrode contact may also affect the performance of polymer-based solar cells. The metal-insulator metal (MIM) model indicates that the Voc is determined by the difference between the work functions of the anode and cathode for a single component diode. As long as one or both of the connections are non-Ohmic, this holds true. The Fermi level of either electrode pins at the proper energy level if the work function of that electrode coincides with or is less than the LUMO or larger than the semiconductor's highest occupied molecular orbital (HOMO). The Voc cannot surpass the polymer's band-gap under these circumstances. With the addition of an electron acceptor material to a BHJ system, however, Voc is restricted to the

difference between the donor's HOMO and the acceptor's LUMO. The annealing duration, in addition to the annealing temperature, may affect the ultimate performance of polymer-based solar cells. The device was investigated with a blend ratio of 1:0.7, thickness of 200 nm, and annealing temperature of 160 C, based on prior optimization of the BHJ blend ratio, BHJ film thickness, and annealing temperature. Voc increases from 0.60 V to 0.62 V and changes from 9.5 mA/cm2 to 10.3 mA/cm2 in inverted devices after 60 minutes of annealing. When the active layer is not annealed, the fill factor is shown to be sensitive to the annealing duration, with fill factors lower than 45 percent. The fill factor rises to 57 percent after 1 minute of annealing and to over 65 percent after 5 minutes of thermal annealing. The PCE exhibited optimal performance after 10 minutes of annealing, with efficiencies of over 4%.

CONCLUSION

In conclusion, as compared to the traditional device design, the inverted device architecture is a potential architecture for the creation of a more perfect polymer-based solar cell. This design enables solution processing methods to deposit the different layers onto flexible substrates, enabling them to be processed using industrial roll-to-roll manufacturing processes. Furthermore, owing to the use of higher work function metals as the top electrode, the inverted device design is more stable to ambient. These greater work function electrodes also allow for the possibility of printing and coating the top metal electrode, which will assist to reduce manufacturing costs. An integrated engineering strategy is presented for developing materials, devices, and improving interfaces and processing to enhance inverted solar cell performance. Inverted solar cells using amorphous fullerenes in the BHJ active layer showed better thermal and morphological stability when compared to devices with PCBM. The inverted architecture's metal oxide interfaces (ZnO, TiO2) were enhanced by utilizing self assembled monolayers, which helped to improve the charge transfer characteristics at the interface as well as the bulk-heterojunction morphology, resulting in high efficiency solar cells. The possibility of creating roll-to-roll solar cell manufacturing is shown using solution processed electrodes to replace vacuum deposited metal electrodes and costly ITO electrodes in inverted solar cells. In order for polymer-based sun cells to be manufactured in large-scale production, further study into the development of the inverted solar cell device design is needed to increase efficiency and roll-to-roll type processibility.

REFERENCES

[1] R. C. Chiechi, R. W. A. Havenith, J. C. Hummelen, L. J. A. Koster, and M. A. Loi, "Modern plastic solar cells: Materials, mechanisms and modeling," *Materials Today*. 2013, doi: 10.1016/j.mattod.2013.07.003.

[2] W. Meng *et al.*, "Conductivity Enhancement of PEDOT:PSS Films via Phosphoric Acid Treatment for Flexible All-Plastic Solar Cells," *ACS Appl. Mater. Interfaces*, 2015, doi: 10.1021/acsami.5b03309.

[3] C. J. Brabec *et al.*, "Origin of the open circuit voltage of plastic solar cells," *Adv. Funtional Mater.*, 2001, doi: 10.1002/1616-3028(200110)11:5<374::AID-ADFM374>3.0.CO;2-W.

[4] Y. Zhou, T. M. Khan, J. W. Shim, A. Dindar, C. Fuentes-Hernandez, and B. Kippelen, "All-plastic solar cells with a high photovoltaic dynamic range," *J. Mater. Chem. A*, 2014, doi: 10.1039/c3ta15073a.

[5] S. E. Shaheen, R. Radspinner, N. Peyghambarian, and G. E. Jabbour, "Fabrication of bulk heterojunction plastic solar cells by screen printing," *Appl. Phys. Lett.*, 2001, doi: 10.1063/1.1413501.

[6] J. Peet, M. L. Senatore, A. J. Heeger, and G. C. Bazan, "The role of processing in the fabrication and optimization of plastic solar cells," *Adv. Mater.*, 2009, doi: 10.1002/adma.200802559.

[7] Y. Wang *et al.*, "Semitransparent, non-fullerene and flexible all-plastic solar cells," *Polymer (Guildf).*, 2016, doi: 10.1016/j.polymer.2016.11.015.

[8]   J. Peet, A. J. Heeger, and G. C. Bazan, "'Plastic' solar cells: Self-assembly of bulk heterojunction nanomaterials by spontaneous phase separation," *Acc. Chem. Res.*, 2009, doi: 10.1021/ar900065j.

[9]   K. M. Lee *et al.*, "Co-sensitization promoted light harvesting for plastic dye-sensitized solar cells," *J. Power Sources*, 2011, doi: 10.1016/j.jpowsour.2010.10.041.

[10]   T. Jeranko, H. Tributsch, N. S. Sariciftci, and J. C. Hummelen, "Patterns of efficiency and degradation of composite polymer solar cells," *Sol. Energy Mater. Sol. Cells*, 2004, doi: 10.1016/j.solmat.2004.02.028.