Efficiency Improvement of Bulk Heterojunction Organic Photovoltaic Solar Cell through Device Architecture Modification

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Abstract-Fundamentally, the overall power conversion efficiency of bulk heterojunction organic photovoltaic (OPV) solar cell depends on two key parameters: (a) the introduction of diverse organic materials as well as their miscellaneous combination as donor and acceptor in the active layer, and (b) the application of ameliorated solar cell device architecture. Here, we demonstrate a different structural design of an organic solar cell device, named textured OPV cell, which offers opportunities to enrich the value of major efficiency parameters, i.e., absorption efficiency, exciton diffusion efficiency, and charge collection efficiency. The proposed redesigned solar cell device structure has several advantages: (i) it absorbs more sunlight and hence creates more photoexcitons, (ii) it virtually increases the active layer thickness that amplifies absorption efficiency, (iii) it increases the distance between exciton generation site and dissociation site and therefore boosts exciton diffusion efficiency, and (iii) it partially effects charge collection efficiency by creating a percolating pathway for the hole and electron transporting phase to the corresponding electrodes. An analytical analysis shows that the proposed device model increases the absorption efficiency about 11-13%, exciton diffusion efficiency about 10% and these changes offer an increment in the overall power conversion efficiency by about 15-20%.

Index Terms—Absorption efficiency, exciton diffusion efficiency, charge collection efficiency.

I. INTRODUCTION

Worldwide renewable energy research and development sectors have been experienced a great variety of experiments during its journey since last three decades or so with a view to producing a reliable and cheap technology that can be a spirited alternative to the conventional inorganic solar cell technology [1], [2]. The state-of-the-art crystalline inorganic silicon based thin film solar cell has already achieved a satisfactory efficiency level, that is $\eta_P \approx 24-25\%$, however, this achievement couldn't unlock the entrance of universal

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PV revolution in spite of the increasing global green energy demand due to the expensive characteristics of inorganic solar cell production [3]. That is why it has become an absolute necessary to find an optimal technology that can ensure the fabrication of a solar cell prototype with low cost consumption facilities. The acclivity of PV research pace in recent years delineates that it's none other organic solar cell technology, one of the better 3rd generation solar cell knowledge that shows a promising character in aspect of efficiency and cost, is going to dominate the global solar cell mass production in the upcoming future [4]. Meanwhile, a number of ideas have been reported based on the discussion about either choosing the better combination of organic materials to develop the internal building blocks of PV device or finding different device architectures, that can fulfill the major demands i.e., enhanced efficiency, moderate lifetime and reasonable cost [2], [5], [6], [16], [18].

The concept of inorganic materials, such as, Si (wafer Si, a-Si, c-Si), CdTe, CdS, GaAs, CIGS, Cu(In,Ga)Se₂, comes from physics, whereas, the idea of organic materials, such as, PCBM, P3HT, C₆₀, CuPc, SnPc, SubPc, MDMO-PPV, PFB, PTCBI, PEDOT:PSS, comes from chemistry. By default, we cannot introduce too much change in the characteristics of the inorganic materials but the organic one. Because of the involvement of various sensitive chemical processes, it is complex to fabricate the organic materials; however, they offer more flexibilities than the inorganic counterparts. That's why, in spite of all sort of complexities, nowadays, the PV researchers are very keen to share their time behind the development of diverse organic materials.

II. BASIC OPERATING PRINCIPLE OF OPV TECHNOLOGY

The basic operating principle of OPV technology is little more complex in comparison with the traditional IPV solar technology. Complexities associated with OPV cell working procedure include four major steps to cover in order to produce electricity from incident solar light. These essential steps are: 1) absorption of sunlight (photon) and hence creation of photoexcitons, 2) Exciton diffusion at the dissociation site, 3) Charge transport, and 4) Charge collection at the corresponding electrodes.

III. EFFICIENCY CALCULATION IN ORGANIC SOLAR CELL

The efficiency of a solar device can be calculated in terms of (i) quantum efficiency (based on device concept) and (ii) IV characteristics (based on circuit analysis).

A. Based on Device Concept

Based on the device concept, the efficiency of organic solar cell can be calculated as follows [9]:

Power conversion efficiency \propto external quantum efficiency

$$=> \eta_{p} \propto \eta_{EQE}$$
$$=> \eta_{p} = \kappa_{p} * \eta_{EQE}$$
$$=> \eta_{p} = \kappa_{p} * \eta_{A} * \eta \text{ int}$$
$$=> \eta_{p} = \kappa_{p} * \eta_{A} * \eta_{ED} * \eta_{CT} * \eta_{CC}$$
(1)

where κ_p = power conversion constant, η_A = absorption efficiency, η_{ED} = exciton diffusion efficiency, η_{CT} = charge transfer efficiency, η_{CC} = charge collection efficiency.

B. Based on the IV Characteristics of PV cell

Based on the IV characteristics of PV cell, the efficiency of Organic solar cell can be calculated as follows [2], [10], [11]:

$$\eta_{p} = \frac{P_{out}}{P_{in}} = \frac{P_{max}}{P_{light}} = \frac{I_{m \ pp} V_{mpp}}{P_{light}}$$
$$= \frac{I_{sc} * V_{oc} * (FF)}{IT * A_{c}}$$
(2)

where P_{out} = actual maximum obtainable power=maximum power point= $I_{mpp} \times V_{mpp}$; I_T = incident solar flux; A_C = area of the cell; Fill Factor (FF) = the ratio (given as percent) of the actual maximum obtainable power to the theoretical (not actually obtainable) power [11]. That is,

$$FF = \frac{\mathrm{Im} \, pp * V mpp}{Isc * V oc} \tag{3}$$

In this article, we would like to demonstrate how our proposed device model affects the increment of power conversion efficiency in respect of device concept by upgrading the value of its quantum efficiency parameters. This is because there is a direct relationship between quantum efficiency and power conversion efficiency: the greater the quantum efficiency, the higher the power conversion rate.

IV. ABSORPTION EFFICIENCY

Absorption efficiency, that is the ratio between how much light is absorbed with how much light is harvested, mainly depends upon the absorption spectra of the organic materials [12],[17]. From the basic operating principle of OPV cell, it is clear that we have to capture more sunlight to produce more photoexcitons. When sunlight falls upon the PV device, roughly three different kinds of situations (Fig. 1) may occur such that: (a) sunlight may be absorbed by the device (b) sunlight may be reflected (c) sunlight may be passed through the device. Among the above incidents, option (a) is a beneficiary event because only in this case sunlight is utilized; however, option (b) and option (c) are not. Because of the very smooth absorption surface of the PV device nowadays we use, a huge percentage of the incident solar light either reflects away or passes through the device indicating a great lose (Fig. 1) with respect to obtain enhanced absorption efficiency.



Fig. 1. Structure of conventional OPV device with sunlight response status.

To solve such problem, we propose to create the absorption surface rough in a very controlled and calculated way (Fig. 2) that can minimize the possibility of sunlight reflection. The smooth surface can be made rough through the process named "texturing" [13]. As a result, the proposed device model allows primary absorption as well as secondary absorption. The incident solar light is absorbed primarily for the 1st time when it falls on the device and then the light is absorbed again during its back reflection, which is called secondary absorption (Fig. 2). Thus, the proposed structure, which is made of textured surface, certainly creates an opportunity to utilize more sunlight. This is because it allows absorbing more sunlight, and hence creating more photoexcitons than the conventional smooth surface structure.

High absorption coefficients (typically exceeding 10^5 cm⁻¹) are one of the inherited advantages of the organic semiconductor materials, which offer to achieve enhanced absorption in even <100 nm thin devices, whereas, large band gap is one of the foremost bottlenecks of them [2]. Studies show that, the inorganic materials, where the band gap is moderate (1.1-1.3 eV), are capable of absorbing about 80-70% of the solar irradiation on earth, however, in case of organic materials, where minimum band gap hovers around 2.0 eV, the capability of absorbing sunlight is only about 30% [14]. Studies upon performance issue of the solar device depict that, in case of IPV cell, power conversion rate is about 0.324%/unit sunlight absorption, whereas, in case of OPV cell, this rate is about 0.2%/unit sunlight absorption. The estimation brings our attention to the point: we can obtain the power conversion efficiency of OPV cell up to 9-10% even with the limited sunlight absorption capacity of organic materials (30%) if an efficient power conversion system is applied. Till today, it is believed that introduction of industrial production of organic solar cell demands at least 10% power conversion efficiency [4].



Fig. 2.Structure of absorption surface of proposed "textured OPV device" with sunlight response.

Absorption efficiency (η_A) in an OPV cell can be calculated using the following formula [15]:

$$\eta_A = 1 - \exp\left(-\frac{L}{L_A}\right) \tag{4}$$

where, L= active layer thickness of the PV cell, L_A = the optical absorption length.

However, according to proposed textured model (Fig. 2), we modify the formula in the following way:

$$\eta_A = 1 - \exp\left(-\frac{L_t}{L_A}\right) \tag{5}$$

where, Active layer thickness of the PV cell after texturing, $L_t = L+d$, the height of the pyramid, $d=L_0$ (tan θ), the unit length of the base of the triangle, $L_0 = \frac{W}{N} \frac{1}{2} = \frac{W}{2N}$ (since, each pyramid (triangle) consists of two triangles) (Fig. 3), W =total width of the solar cell, N= the number of pyramid.

V. EXCITON DIFFUSION EFFICIENCY

The separation of photoexcitons into free charge carriers, which is considered as the most significant part of the entire working procedure of OPV, takes place in the exciton diffusion step. Basic operating principle of OPV technology depicts that once the photoexciton is generated inside the active layer upon absorption of sunlight it needs to be diffused at the donor-acceptor (D/A) interface to free the charge carriers. The exciton diffusion step is involved not only in the process of splitting up the photoexcitons into free charge carriers, which are collected at the corresponding electrodes. That is why, how much charge will be received at the receiving end (corresponding electrodes) basically depends upon how much free charges are generated through successful diffusion process.

The matter of concerned, however, is that there are a number of loss mechanisms that account for abortive diffusion of photoexcitons at a large scale due to the inherited drawbacks of bulk heterojunction structure and the complexity of basic operating principle of the OPV technology. In addition, recombination process is one of the chief impediments for an exciton to dissociate properly. Such limiting factors are responsible greatly for lessening the possibility of splitting up the photoexcitons into free charge carriers to about only 10%, which is conceived as one of the major obstacles for obtaining a better overall power conversion rate from an OPV device [10]. Therefore, it has become a key challenge for the OPV researchers nowadays to find out solutions that can be applied to lessen the lose mechanisms during exciton diffusion process. For the researchers, the short listed key challenges are: (a) to protect the photoexcitons from being recombined before splitting up, (b) to generate photoexcitons with moderate exciton diffusion length, and (c) to ensure the best use of limited lifetime of the photoexcitons.

In order to resolving such confronts, here we propose to moderate the structural design of the conventional OPV cell according to Fig.4. In this case, the active layer as well as the other layers are highly folded in one another such a way that the excitons can be formed as near as possible to the dissociation site. As a result, the short exciton diffusion length as well as the limited span of lifetime of the photoexcitons can be employed more efficiently. This is because the suggested triangular textured model offers the potential to cut the travelling distance for an exciton from its generation site to dissociation site and hence reduce the recombination losses. And finally the complete structure of the proposed triangular textured OPV device will look like Fig. 5.

Exciton diffusion efficiency is the fraction of photogenerated excitons that reaches a D/A interface before recombining. It is alleged that the chief parameters that run exciton diffusion process are basically (i) exciton generation length-the distance between exciton generation site and dissociation site and (ii) exciton diffusion length-the minimum required distance that has to be travelled by the exciton to split up. The exciton generation site adverts to the place where the exciton forms after sunlight absorption which is basically depends on the optical absorption length of organic materials.

Here, we propose a formula for calculating the exciton diffusion efficiency:

$$\eta_{ED} = 1 - \exp\left(-\frac{L_{EG}}{L_{ED}}\right) \tag{6}$$

where, exciton generation length, $L_{EG} = L_{DS} - L_A$, L_{DS} = Dissociation site length (with respect to anode), L_A = optical absorption length. Here, $L_{DS} > L_A$ (since optical absorption length cannot exceed dissociation site length). The proposed equation affirms the key concepts of the exciton dissociation occurrence, such as, (i) the exciton diffusion efficiency decreases if the exciton diffusion length increases and vice versa (ii) the exciton diffusion rate increases with the increment of exciton generation length.



Fig. 3. Structure of absorption surface of proposed model after texturing.

On the other hand, exciton diffusion efficiency can be described as the ratio between the number of electrons leaving the device under short circuit condition per time per area and the number of photons incident per time and area [11]. This is termed as incident photon to converted electron efficiency (IPCE). It can be expressed as follows [10], [11]:

$$IPCE = \frac{\text{no. of extracted electrons}}{\text{no. of incident electrons}}$$
(7)

$$=\frac{1240*Isc}{\lambda*Pin}$$
(8)

where, $\lambda[nm]$ = incident photon wavelength, $I_{sc}[\mu A/cm^2]$ = photocurrent of the PV device. IPCE is regarded as one of the core parameters of external quantum efficiency, which includes few lose mechanisms like losses due to reflection at the surface, transmission through the PV device [11].



Fig. 4. Complete device structure of the proposed textured OPV solar cell with working procedure of active layer.



Fig. 5. Proposed textured OPV solar cell architecture.

VI. CHARGE TRANSFER AND COLLECTION EFFICIENCY

At the final stage of the operation process of OPV, the free charges are collected at the corresponding electrodes. This segment, perhaps, is the most tranquil one where we experience least system loses. The discovery of bulk heterojunction structure offered the improvements for successful advent of free charge carriers to their subsequent electrodes. The foremost parameters that drive this process are applied voltage (V) and mixed layer thickness (d_m).

The carrier collection efficiency is the probability that a free charge carrier, generated at the D/A interface by fruitful dissociation of an exciton, reaches its corresponding electrodes. It can be defined as follows [16]:

$$\eta_{CC} = \frac{L_c(V)}{d_m} \left[1 - \exp\left(-\frac{d_m}{L_c(V)}\right) \right] \tag{8}$$

Here, V=applied voltage, d_m =mixed layer thickness, charge collection length, $L_c(V) = \frac{L_{c0}(V_{bi} - V)}{V}$, Lc_0 =a constant,

 V_{bi} =built-in-potential. We see that, $\eta_{CC} \approx 1$ when $d_m \ll$

$$L_c$$
 and $\eta_{cc} \approx \frac{L_c(V)}{d_m} \ll 1$ when $d_m \gg L_c$ [16].

VII. RESULTS AND SIMULATIONS

Fig. 6 depicts the changes in absorption efficiency that

takes place based on the thickness of the active region. We see that the higher the active layer thickness, the higher the absorption efficiency.

Fig. 7 illustrates the enhancement in absorption efficiency that is experienced through the proposed textured OPV device model (the dotted line "--") with the use of formula (5) compared to the absorption efficiency of conventional OPV device (the plain line "-") with the use of formula (4). For example, if active layer thickness, L=100nm, optical absorption length, $L_A=90$ nm, η_A (conventional model)=67.08%, whereas, η_A (proposed model)=75.06%, hence, increase in η_A is about 11.9%.

An analytical analysis shows that through the proposed device model of OPV the absorption efficiency rate can be enriched about 12-14% (Fig. 8).



Fig. 6. Dependency of absorption efficiency on active layer thickness.



Fig. 7. Increment in absorption efficiency based on absorption surface style.



Fig. 8. Maximum increment in absorption efficiency after texturing.

In Fig. 9, an analytical analysis (based on the proposed model and using Equation (6)) shows that, we obtain about 7.61% increases in η_{ED} . In addition, the exciton diffusion rate becomes almost saturated after a certain increase of exciton

dissociation site length.

Fig. 10 is an instance of IV characteristics of illuminated and dark current of an OPV device with nth order polyfit function. We observe that, when $n=5(5^{\text{th}} \text{ order polyfit function})$, it best suits the real life data.

Both the changes, we obtain from absorption efficiency and exciton diffusion efficiency in our proposed model, create an opportunity to enhance the overall power conversion efficiency about 17-18%.



Fig. 9. Increment in exciton diffusion efficiency after texturing.



Fig. 10. IV characteristics of OPV solar cell using polyfit function.

VIII. SUMMARY

In summary, we demonstrate an idea to enhance the power conversion efficiency of bulk heterojunction OPV solar cell by changing the device architecture. By engineering the proposed architecture more significantly, we can be in command of the efficiency parameters to work more efficiently. Recently, organic solar cells have crossed the hurdle of 5% power conversion efficiency with the conventional device architecture [17]. We anticipate that the application of our proposed "textured organic solar cell device architecture" create chances to overcome the loss mechanisms of the traditional OPV device. In the near future, modification of established device structures and development of novel new architectures might be the undertaking options in order to obtain high efficient organic PV solar cell.

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