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Simulative Parametric Study on Heterojunction Thin Film Solar Cells Incorporating Interfacial Nanoclusters Layer

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Abstract: Organic solar cells deal with small organic molecules for absorption of light at low cost and high efficiency. In this paper, we have analyzed the photovoltaic (PV) characteristics of double heterojunction solar cell that consists of copper phthalocyanine (CuPc) and 3,4,9,10-perylenetetracarboxylic bis-benzimidazole (PTCBI) thin films. Here, CuPc and PTCBI layers are combined by an interfacial layer consisting of nanoscale dots. Different plasmonic materials (i. e. Ag, Au, and graphene) are selected as alternative nanoscale dot layer to examine their effect on solar cell performance. Further, the solar cell performance is also examined via variation in active layer thickness. The choice of interfacial layer material and variation in active layer thickness offer grounds for future efficient PV cells.

Keywords: CuPc/PTCBI solar cells, energy conversion efficiency, excitons, plasmonic materials

Introduction

Being an alternative to continuous depleting conventional energy sources, solar energy has gained tremendous research attention due to its vast availability. Photovoltaic (PV) technology is one of the most popular option to convert the solar energy into electric form. It offers numerous advantages in terms of cost effectiveness, easy fabrication, and environment friendliness. Over the time, the PV technology has been updated from first generation silicon solar cells to second generation thin film solar cells and followed by third generation solar cells such as dye sensitized solar cells, organic solar cells, etc.

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Besides vast market share of silicon solar cells, their complex manufacturing causes to promote the thin film solar cells. The thin film solar cells offer potential benefits in terms of ease of manufacturing and installation flexibility at a cost of somewhat lower energy conversion efficiency (ECE) than that of silicon solar cells. The thin film solar cell consists of two or more thin layers of materials termed as contact, reflector, absorber, hole transport layer, etc. situated on the substrate. There are two different parameters (i. e. light absorption and exciton diffusion) that can affect the performance of organic PV cells. Ideally, the materials should have high quantum efficiency of excited carriers and high optical absorption. The choices are available for absorber material in thin film such as copper indium gallium arsenide (CIGS) and cadmium telluride (CdTe). The use of In and Ga materials in CIGS makes the system complex and also the use of toxic Cd can easily react with environment (Chopra, Paulson, and Dutta 2004). However, it is not practicable to collect all photo generated electrons in thin film PV cell. The recent trends in thin film solar cell deal with variations in their structural design in order to enhance the light absorption. For instance, materials possessing scattering property for photons can be incorporated to enhance the number of incident photons at absorber layer (Kaiser et al. 2001). Thereafter, further improvements deal with the use of organic materials for achieving high ECE at low cost.

Organic PV cell contains donor and acceptor material. In case of heterojunction solar cells multiple donor-acceptor pairs are stacked together to enhance the light absorption. The stacking of donor-acceptor pairs can be achieved via direct or indirect approaches. The direct method basically deals with series connection of sub-cells without any separation or interfacial layer (Hadipour, de Boer, and Blom 2008). On the other side, indirect approaches involve the use of interfacial layers for connection between the sub cells. The heterojunction solar cell containing p-type cupric oxide (CuO) absorber material followed by n-type Zinc oxide (ZnO) offered a maximum ECE of 0.08 % (Dimopoulos et al. 2013). The concept of nano-cluster layer in organic PV cells is recently introduced to lower the recombination of the charge carriers at the interface (Peumans, Yakimov, and Forrest 2003). Furthermore, the interfacial layer can also help in enhancing the optical field thereby supporting the increased absorption in the active layer (Rand, Peumans, and Forrest 2004). Between adjacent cells, the nano-cluster layer generates multiple excitons during light absorption. These excitons can be dissociated at the metallic interface layer with the help of electric field. Due to small diffusion length of excitons, the dissociation process should be carried out at the interface of donor and acceptor. To achieve high efficiency, these excitons should be dissociated in free charge carrier. Furthermore, surface plasmonic layers can enhance the electromagnetic field that can contribute in performance improvement of solar cells (Raether 1988). The incorporation of Ag-based plasmonic layer offered enhancement in optical field that resulted in increased ECE (i. e. 2.2 %) of the organic solar cell than that of without plasmonic layer (i. e. 1.3 %) (Morfa et al. 2008). In another study, two, three and more stacked thin heterojunction have been reported with interfacial layer of Ag clusters and offered an ECE of the device was 2.5 % (Yakimov and Forrest 2002).

The plasmonic behaviour of Ag or Au promotes their use as inter electrodes. The insertion of inter electrode depend upon the sequence of organic layer in heterojunction cell. The CuPc/PTCBI structure with Ag inter electrode offered a V_{oc} of 1.35–1.5 V (Triyana et al. 2004). The limitations in terms of low ECE motivate researchers to explore the role of these nano-cluster layers more effectively.

In this paper, we realized the double heterojunction cell structure using CuPc/PTCBI materials. The choice of different materials is evaluated at the interfacial layer to optimize their effect on the performance of heterojunction structure. This paper is organized as introduction (refer to Section 1), proposed parameters of heterojunction solar cell (refer to Section 2), results and discussion (refer to Section 3) and conclusion (refer to Section 4).

Proposed Parameter of Heterojunction Photovoltaic Cell

PV cells with multiple p-n junctions produce leading current at different wavelengths of light. This leading current is important for series resistance effect, especially from the emitter that affects the operating point by varying it in biased condition. The modeling of the heterojunction structure can be done by two or three dimensional approaches. But three dimensional approach makes system more complex, time consuming and somewhat difficult to simulate. Here two dimensional approach is used to design the heterojunction for obtaining the J-V curve and quantam efficiency.

The device structure considered in this paper includes CuPc and PTCBI materials as donor and acceptor respectively, as shown in Figure 1 (Rand, Peumans, and Forrest 2004). Each sub-cell consists of CuPc and PTCBI layers in a heterojunction configuration. The plasmonic nano dots interlayer embedded between the sub-cells enhances the electric field due to surface plasmon. The main reason of taking up of front sub cell layer of CuPc material is its high absorption property and is followed by the PTCBI material due to planner interface property. A silver reflector is placed at the back of the cell that collects the electrons and a layer of indium tin oxide (ITO) is deposited on the front of cell that behaves as cathode. The series connection of the sub cells increases the short circuit current density (J_{sc}) of the cell which further decreases the series resistance and thereby enhancing the ECE of the cell.

In the model, PV cells are fabricated on the ITO substrate. ITO is mostly used as transparent oxide layers due to its attractive properties in terms of optical transparency and electrical conductivity. Due to its transparency, it increases the concentration of charge carriers and therefore the conductivity is also increased. The substrate ITO thickness is taken as 0.15 µm. In first sub cell (PV1), the thickness of donor layer is 0.015 µm and acceptor layer is 0.013 µm. The second sub cell (PV2) is designed above the interfacial plasmonic layer. The sequence of donor and acceptor layer in PV2 cell is kept same but the thickness of the layers is varied because balance of light absorption by each sub cell is important, so that thickness of layers should be rearranged to find out the optimum conditions for ECE and solar cell thickness. The thickness of donor layer in PV2 is kept 0.013 µm, whereas acceptor layer thickness is fixed to 0.03 µm. At the back, silver is used as a back reflector having a thickness of 0.1 µm.

In heterojunction solar cell, photons having higher energy than active layer band gap are absorbed by the active layer (donor and acceptor layer). They get converted into excitons upon their absorption. Due to repulsive columbic forces, particles in conduction and valance band effectively attract each other. These excitons are generated on each organic layer and they start moving towards the interface. The holes from PV1 and electrons from PV2 are collected directly by the ITO and Ag electrode, respectively. At the same time unpaired electrons from the PV1 and holes from PV2 move towards the internal electrode for recombination. The nano clusters can generate an additional electric field (Kim, So, and Moon 2007) due to the recombination of unpaired charged particles which are produced internally. The enhancement in electromagnetic field with the surface plasmon, photogenertation of excitons will be more in the donor than in the acceptor. The unpaired electron transition probability in donor and acceptor materials is directly proportional to the electromagnetic field strength. Thus, the electric field due to plasmon enhances the photon absorption in the cell (Etchegoin et al. 2003) and covers the wide spectral range. As shown in Figure 1, the absorption of light at device originate from the back scattering of the light by nano-clusters, which increases optical length of the device (Liu and Nunzi 2012). This enhancement in optical length improves the light trapping ultimately improving the PV performance of the device. The nano-clusters layer of different materials can be inserted between the heterojunction of the device. The nano-clusters layer works as an efficient unexcited carrier recombination layer.

Results and Discussion

Rsoft Simulator is a CAD based simulation tool, which is used for simulative analysis of solar cell. In our simulation process, standard AM 1.5 radiation of solar spectrum as illumination process was adopted. The 2-D Full Wave Simulation based on the FDTD technique was utilized.

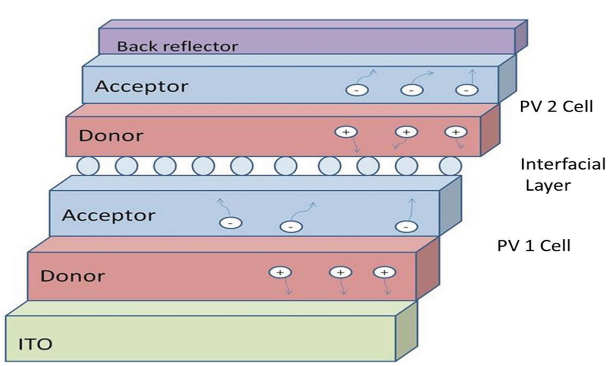

Figure 1: Schematic diagram of double heterojunction thin film solar cell. Nano clusters layer is shown by circles in between the sub cells.The charge carrier recombination occurs at the interfacial layer of device. Dissociation of donor-acceptor interface leads to hole in PV1 and electron in PV2 cell which contribute to photo current and excess electron in PV1 and hole in PV2 recombine at the nano dot interface layer (Rand, Peumans, and Forrest 2004).

Impact of Alternate Interfacial Plasmonic Materials

In this section, we focus on the different materials that can be used at the interface. For better efficiency we have focused on those materials which have low loss in the UV-Vis and near infrared spectral range. The nano structure morphology of the materials has huge influence on the energy conversion performance of the PV cell. The plasmonic application of nano-cluster requires negative permittivity material (Ag, Au and Graphene) which is denoted by negative ε. This permittivity is obtained from only those materials that have high plasmonic frequency than the desired frequency of device or application (West et al. 2010). In our work, we will describe different metals which have high conductivity and large plasmonic frequency. Among all the metals silver and gold are the mostly used metals for the plasmonic purpose.

Silver (Ag) is the most commonly used plasmonic material having high absorption and low loss in the visible and near infrared range. Silver has the smallest damping ratio; damping ratio is defined as summation of damping rates that occurs due to different scattering like: electron-electron scattering, electron-phonon scattering and grain boundary scattering. The size of plasmonic particle can change the grain boundary scattering. Therefore, due to these scattering properties and low damping rate, silver has high optical frequency (West et al. 2010). Silver has been used for negative-refractive index material (Dolling et al. 2007) and high optical transmission property (Ebbesen et al. 1998). Silver faces several challenges in terms of losses due to surface dependent property (Drachev et al. 2008) and also can degrade quickly during fabrication (Lewowski 1995; Wei and Eilers 2009; Oates and Mücklich 2005).

Gold is another best plasmonic material due to its low losses in the visible and NIR ranges. In comparison to silver, gold is expensive but with high chemical stability. Gold has larger damping ratio than silver. Gold has advantage of stability in environment conditions. But it has low NIR frequencies due to that it has high inter band losses at 500 nm. Gold can form a continuous film at thickness around 1.5–7 nm range (So, Fong, and Cheung 2001; Smith et al. 1999; Yagil et al. 1992). During fabrication, thin film is deposited with particular thickness; if the thickness is less than percolation threshold then it forms semi/discontinuous film with different optical properties (Seal et al. 2002).

Recently, graphene has become popular in the recent research community because of its zero band-gap structure and high carrier mobility properties (Novoselov et al. 2004, 2005; Emtsev et al. 2009). Graphene also has plasmonic property at the metal/dielectric interface. In graphene, inter band transitions occur above the threshold which is determined by Fermi energy level. But inter band transition contributes to losses because of zero band gap structure material. Below threshold value, the losses are obtained due to impurity scattering. It also suffers from losses during relaxations times.

The selection of plasmonic materials (i.e. Ag, Au and Graphene) for interfacial nano-cluster layer in heterojunction solar cell can affect their performance, as shown in Table 1.

Table 1: Simulative results of heterojunction solar cell for different nano-cluster plasmonic materials.

Heterojunction Solar Cell Structure (length in μm)	η(%)
ITO (0.15)/CuPc (0.015)/PTCBI (0.013)/**Ag nano dots (0.1)**/CuPc (0.013)/PTCBI (0.03)/Ag (0.1)	**4.01**
ITO (0.15)/CuPc (0.015)/PTCBI (0.013)/**Au nano dots (0.1)**/PTCBI (0.013)/CuPc (0.03)/Ag (0.1)	**3.71**
ITO (0.15)/CuPc (0.015)/PTCBI (0.013)/**Graphene nano dots (0.1)**/CuPc (0.013)/PTCBI (0.03)/Ag (0.1)	**3.12**

The heterojunction structure is simulated by using inter-layer of either silver, gold or graphene that gives efficiency of 4.01 %, 3.71 % and 3.12 %, respectively. To get the better efficiency, the silver nano-cluster layer can be used due to its high absorption and low losses plasmonic properties.

Impact of Absorber Layer Thickness

The influence of absorber layer thickness on performance is investigated for this device structure for obtaining better device performance. With increase in device thickness from 0.008 μm to 0.015 μm, the overall increment in the majority carrier at the absorber layer can be observed that ultimately enhances the ECE.

The effect of variation in thickness of CuPc material is analyzed through simulation, refer to Table 2. The CuPc thickness is varied in the range of 8–15 nm to investigate its effect on the performance of cell.

The variation in thickness of donor layer (8–15 μm) helps in optimizing the best conditions for PV performance. We obtained maximum efficiency at 0.015 μm thickness of CuPc layer because thickness of device should be equal to diffusion length which increases the absorption capability of device.

Table 2: Simulative results at different thickness of active layer.

Donor (PV1 Thickness μm)	η (%)
0.015	4.01
0.012	3.96
0.01	3.92
0.008	3.88

Comparison between Present Work and Reported Ones

In already reported heterojunction PV cell (Rand, Peumans, and Forrest 2004), the experimentally obtained efficiency of the cell is 2.5 %. To achieve further improvements in energy conversion efficiency (ECE), we hereby optimize the various parameters like different materials for nano-cluster and thickness of active layer.

The comparison between the reported and present work is shown in Table 3. We found that the increase in thickness of absorber material can help in attaining the high efficiency of the device.

Table 3: Comparison between reported and present work.

Heterojunction Solar Cell Structure Parameters (thickness in μm)	η (%)	Ref.
ITO (0.15)/**CuPc (0.01)**/PTCBI (0.013)/Ag dot (0.001)/CuPc (0.013)/PTCBI (0.03)/Ag (0.1)	2.5	(Rand, Peumans, and Forrest 2004)
ITO (0.15)/**CuPc (0.015)**/ PTCBI (0.013)/Ag dot (0.001)/CuPc (0.013)/PTCBI (0.03)/Ag (0.1)	4.01	This work

Figure 2 shows the J-V curve after simulating the present work. This efficiency is approximately double (4.01 %) in comparison to literature (Rand, Peumans, and Forrest 2004) along with a short current density of 44.3865A/m^2. The increase in short circuit current density can be attributed to the reduction in series resistance of device. As the number of absorbed photons increases in the device, it ultimately causes an increase in the number of photogenerated electrons in the structure as well as

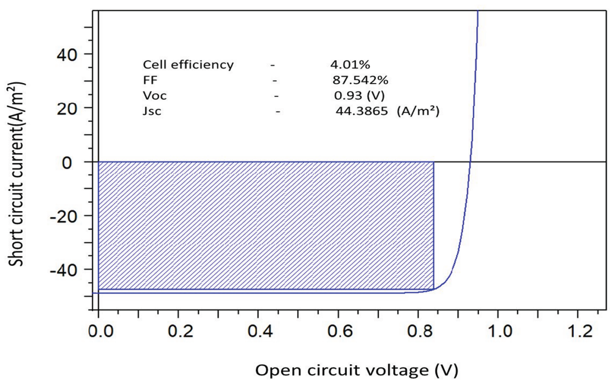

Figure 2: Simulated graph of short circuit current density versus open circuit voltage for the photovoltaic device (present work). The shaded rectangle represents the fill factor. Here V_{oc} denotes the open circuit voltage, I_{sc} denotes the short circuit, and FF denotes the fill factor.

current density of the device. The Fill factor (FF) of the present work is found to be 87.54 % which is quite high than that of reported work (i. e. 55 %).

Conclusion

The purpose of this work is to optimize the different parameters to improve efficiency of heterojunction thin film solar cells. Through the Full Wave Rsoft solar cell utility simulator, we designed a CuPc/PTCBI double heterojunction structure. At optimum conditions, the device provides a higher ECE of 4.01 % that can be attributed to the increased optical absorption of the incident photons. A significant rise in absorption is observed at 0.015 μm thickness in comparison to 0.01 μm thickness of CuPc material. The silver plasmonic nano-cluster material interlayer is inserted between sub cells. This shows that not only thickness of CuPc material influences the photon absorption, but the choice of plasmonic materials also has a significant effect on the efficiency. The increase in photons absorption by absorber material lead to increased short circuit current density. Further improvement in the cell performance of heterojunction can be approached by optimizing several parameters such as variation in diameter of nano dots, use of tandem geometries, etc.

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