Optik 125 (2014) 644–650

Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.de/ijleo

Wavelength comparison study for photocurrent and thickness in organic tandem solar cell with PF10TBT:PCBM by computational simulation

Maryam Namvar[a,*], Madiheh Namvar[b], Seyed Mohammad Bagher Ghorashi[c], Adeleh Mohamadi[d]

[a] Atomic & Molecular Group, Faculty of Physics, Yazd University, Yazd, Iran
[b] Department of Physics, Science and Research Branch, Islamic Azad University, Tehran, Iran
[c] Department of Photonics, Faculty of Physics, University of Kashan, Iran
[d] Electronic Engineering, Leuven University, Belgium

ARTICLE INFO

Article history:
Received 25 February 2013
Accepted 1 July 2013

Keywords:
Computer simulation
Tandem solar cells
Optical modeling

ABSTRACT

In this work, we have been investigating an organic tandem solar cells composed of PF10TBT:PCBM by using optical modeling and simulation method to investigate the correlation between thickness and photocurrent. Possible thickness pairs of tandem cell are provided when front layer and back layer absorb same amount of photons. In order to obtain the possible thickness pairs for different wavelengths, photocurrent has been simulated as function of back and front layer thickness. Energy dissipation in term of distance along cell and wavelengths were analyzed to interpret the optimal geometry of tandem cell. In order to find the appropriate materials for maximum efficiency, energy dissipation as function of optical constant (n) and wavelengths were simulated to derive the optimal condition.

1. Introduction

Photovoltaic cells based on organic materials have been a hot issue, since they are expected to offer inexpensive and flexible light–electric energy conversion tools, which can be used to replace conventional silicon-based solar cells [1–3]. Unfortunately, these materials demonstrate less than ideal optical absorption in the visual range. A partial solution to this problem has been to exchange polymers with low-band gap (LBG) alternatives in the active layer and collect a broader portion of the solar spectrum that includes longer wavelengths of light [4,5]. This technique has shown some improvement in efficiency, but not as much as would be necessary to enable organics to compete with inorganic photovoltaic. The next logical progression has been to combine the best properties of each type of cell into either series or parallel tandem structures so that the broadest possible spectral content could be captured [6–8]. The fabrication of stacked organic solar cells based on a series connection of two cells has been achieved by using an ultrathin metal layer as a recombination center between the individual cells to enhance electron injection and to reduce the contact resistance. When this serial configuration is used, it is expected that the open-circuit voltage of tandem cell is equal to the sum of open-circuit voltage of each sub-cell. However, the short-circuit current density of tandem cell is rather complicated to predict from short-circuit current density of individual sub-cells because it depends largely upon the thickness of active layers [9]. It is known that the optimal thickness of the active layer for the maximal performance of OPV exists in the single cell mainly due to the trade-off effect between the light absorption and the charge carrier recombination [10]. The most direct way to increase absorption is increasing the thickness of the photoactive layer [11]. However, lower photocurrent in active layer device by thickness enhancement can be attributed to the electric filed inside the active layer which decreases at the constant bias voltage. Since the exciton dissociation rate depends on the electric field, the dissociation rate of excitons becomes smaller at lower electric field. Another possible reason for the decrease of short-circuit current density in thicker active layer is an increase in the recombination rate. Since a thicker device has longer pathway for charge collection, it is easily expected that the probability for separated charges to recombine increases. Furthermore, due to lower electric field within thicker device under the short-circuit condition, the drift of charge carriers becomes slower and therefore the chance of recombination would be increased [12]. Therefore, thickness of active layers can play a crucial role in overall device performance, optically as well as electrically. Many numerical and simulation research

* Corresponding author. Tel.: +98 5842254843.
E-mail address: maryamnamvar@rocketmail.com (M. Namvar).

0030-4026/$ – see front matter
http://dx.doi.org/10.1016/j.ijleo.2013.07.086

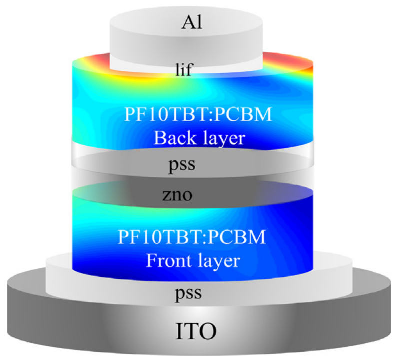

Fig. 1. Schematic representation of organic tandem solar cells based on PF10TBT:PCBM.

have been accomplished on operating mechanisms and design of optimal device geometry in tandem cell [13–17]. The absorption of light affected by active layer thickness within these multilayer devices is one of the crucial optical processes; therefore it is one of the main areas of numerical simulations.

In this report, we have presented a computational approach in the organic tandem solar cells that is based on optical modeling. We have considered on correlation between photocurrent (G_{ph}), light absorption and active layer thickness and investigated the optimized geometry for organic tandem photovoltaic cells based on PF10TBT:PCBM that was fabricated by Moet et al. [11]. The geometry of the tandem cell and intermediated layers are shown in Fig. 1. Due to its almost constant refractive index throughout the whole visible sunlight spectrum, the covering glass only decreases the amount of light absorption, but does not affect the location of the maximum and minimum of the absorption density inside the photovoltaic device. For that reason we did not consider the glass in our calculations [18]. As an input to the optical modeling, the optical constants (k, n) of materials were taken from the literature [12,19–21].

2. Theory

Optical simulation of the absorption in organic tandem solar cells has been performed using techniques that employ the transfer matrix method (TMM). Transfer matrix formalism has been used by Pettersson et al. [22] to calculate the absorbed optical energy within the multilayer structure. This formalism is widely used to optimize layer structures for single junction as well as tandem cell [23–27]. In this study we present a comprehensive numerical model which considers optical parameters of OPV cells consist of a multilayer structure, with layer thicknesses on the order of the wavelength of the incident light. When a plane wave incident from the ambient side propagates through the layers of device toward the substrate side, the optical electric fields at the position z can be represented by the system transfer matrix. The optical modeling and simulation theory with details can be explained in [22,28–30] but in brief, we have described calculations by the knowledge of optical thin film. The time average of the energy dissipated per second in a layer j as a function of distance in depth of cell is described:

$$Q_i(z,\lambda) = \frac{2\pi c\varepsilon_0 k_i n_i |E_i(z,\lambda)|^2}{\lambda} \tag{1}$$

The variable z represents the position inside the solar cell when waves travel perpendicularly through the device layers. Density of photons absorbed per second can be derived via:

$$n_{\text{photons}} = \frac{\alpha I \lambda}{hc} \tag{2}$$

where

$$I = \frac{n}{n_0}|E_{\text{norm}}|^2 I_0 \tag{3}$$

where α stands for absorption coefficient which is given by $\alpha = \frac{4\pi k}{\lambda}$, and k stands for the imaginary part of the refractive index. An optical model based on the transfer matrix method was used to calculate the time-rate of absorbed photons in the two photoactive sub cells. The time-rate of absorbed photons values in individual cells are converted into photocurrent densities (J_{ph}) for each of the combined sets of sub cell thicknesses under study [26]. Note that the time-rate of absorbed photons depends on optical interactions in all the layers of the tandem design. The complex indices of refraction for each of the layered materials are used to describe optical transmission, reflection, and absorption characteristics throughout the entire tandem cell. As an input to the optical model, thicknesses of other layers in the device were chosen from the common multi-layer structure of organic tandem polymer solar cells [11] which are composed: ITO (150 nm)/PEDOT:PSS (40 nm)/PF10TBT:PCBM (dfront)/Zno (20 nm)/PEDOT:PSS (30 nm)/PF10TBT:PCBM (dback)/Lif (1 nm)/Al (100 nm). Optimal thicknesses of active layer obtained from [11] experimental work are: PF10TBT:PCBM (100 nm) as front layer and PF10TBT:PCBM (70 nm) as back layer. In addition, light absorption in the top and bottom cells is greatly affected by their thicknesses. The optical analysis was performed over a wavelength range of 300–800 nm based on AM 1.5 G irradiance.

3. Result and discussion

3.1. Photocurrent

To convey the matrix formalism of preceding section into simulation, we now consider on photocurrent which can be balanced with proper design in respect to front and back layer thicknesses by determining possible thickness pairs according to same photon absorption in each sub cell because it is more beneficial to consider the parameters as a function of active layer thicknesses than of other variables according to its various options to study. Before specifying this particular distribution, it is necessary to state that a key feature of the optical process based on the electromagnetic field such as light absorption as the most effective and fundamental process which leads to photocurrent due to dissociation excitons, derives from traveling waves which represent the transport of energy from one point to another.

Simulated photocurrent density values in front and back layer as a function of their thicknesses for wavelengths: 350, 450, 550, 650 nm are illustrated in Fig. 2. The surface which increase along front layer devote the photocurrent in front layer and the surface which increase along back layer devote the photocurrent in back layer. In the case of back layer, two specific peaks for wavelengths: 450, 550 nm were occurred at about 50 and 150 nm along back layer while a secondary peak includes greater value by penetrating into higher thicknesses. For wavelengths: 350, 650 nm, photocurrent demonstrate distinctly ascending rate and peak progressively shift to higher thickness values. There is a tendency for Photocurrent to be lost in back layer along front layer and lose was occurred for higher front layer thickness. In the case of front layer, photocurrent values increase evidently by increasing thickness for all wavelengths. Our particular interest in photocurrent simulated derive from the fact that we proceed to find the possible thickness pairs for front and back layer for some wavelengths. It is sufficient to consider the problem in intersection between two surfaces [10], were two sub cells absorb same amount of photons, and produce same photocurrent. Therefore, these thickness pairs are possible thicknesses for both layers because in tandem device of serial