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Organic Solar Cell: Optics in Smooth and Pyramidal Rough Surface

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Abstract : *The optics in a substrate configuration (n-i-p) thin-film organic solar cell was investigated, where ZnPc:C60(1:1) blend organic photoactive material was sandwiched in between a wide band-gap hole transport layer (MeO-TPD) and an electron transport layer (C60) materials. The study was carried out for optical wave propagation simulation results of upper limit quantum efficiency and short circuit current based on the finite difference time domain method. At first, a smooth substrate solar cell was optimized by observing the influence of the variation of each layer thickness. The optimized flat solar cell achieves 13.65 mA/cm^2 short circuit current with a maximum of 84% quantum efficiency in 640 nm of optical spectrum. Then a light trapping pyramid textured optical model has been proposed for better light trapping, higher diffraction, and enhanced effective thickness, which can lead to more light absorption than organic solar cells on smooth substrates. Finally, the influence of periods and heights on the enhanced effective thickness validated the model.*
Keywords : *Light trapping, n-i-p, MeO:TPD, ZnPc:C60, surface texture.*

I. Introduction

With the synthesis of novel organic molecules and the design of new device structures, the PV efficiency has led to recent and significant improvements in both small molecular weight and polymeric solar cells. Organic semiconductive materials have impressive properties such as simple fabrication, light weight, mechanically flexible, possibility to tune electronic band-gap, environmentally safe, and less toxic manufacturing techniques have made organic solar cells cost effective and advantageous over the conventional silicon solar cells [1]. A better electrical performances can be achieved when the thickness of the active region is limited to less than a hundred of nanometers, since the carrier diffusion length is very low [2]. Up to now, single junction organic solar cells (OSCs) are capable of reaching power conversion efficiencies of about 8% [3], while model calculations predict that it is possible to obtain 10%–11% or even more [4] within blended single layer structures.

In this manuscript, the investigation has been started with the optimization for a smooth substrate organic thin-film solar cell. A finite difference time domain (FDTD) simulation tool (OptiFDTD®) was used to study the wave propagation inside the solar cells, where Maxwell's curl equations were rigorously solved to simulate near-field and far-field wave propagation. Then a light trapping pyramid textured structure has been proposed, which can be used to get an enhanced diffraction of light and higher effective thickness in the device.

II. Smooth Substrate Organic Solar cell

1.1 Optical Simulation Model

A schematic cross section of simulated substrate configuration thin-film organic solar cell on smooth surface is depicted in Fig. 1(a). The solar cell structure, investigated in this study, consists of a 130 nm indium tin oxide (ITO) front contact, followed by a 20 nm hole transport layer, MeO-TPD, a 60 nm photoactive blend material of ZnPc:C60 (1:1), a 35 nm electron transport layer of C60, and a 100 nm Al metal back contact with a 10 nm of TiO2 optical spacer. The structure of the flat solar cell used in this investigation is consistent with the cell developed by the Institut für Angewandte Photophysik Research Group, except an additional TiO2 spacer used for better absorption and conductivity [5].

The complex refractive indices for each layer were used to simulate for the electric field distribution throughout the device structure. The simulations of the optical wave propagation within the solar cell were carried out for wavelengths ranging from 300 nm to 900 nm. From the electric field distribution, power loss for the individual regions of the solar cell were calculated by using the equation (1).

$$Q(x,y) = \frac{1}{2} c \in_0 n\alpha |E(x,y)|^2 \qquad (1)$$

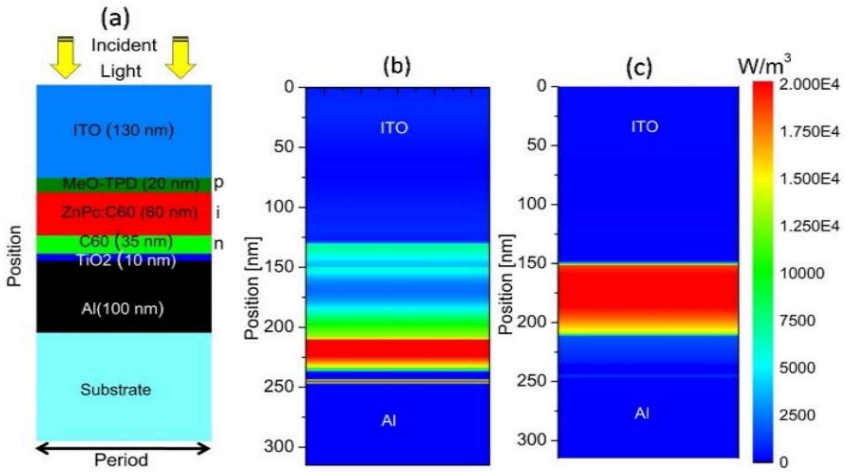

Fig. 1: (a) Schematic cross section of simulated organic solar cell on smooth substrate; corresponding power loss profile for monochromatic illumination of wavelength (b) 400 nm, and (c) 640 nm.

where α is the absorption coefficient, with n being the real part of the complex refractive index, E(x, y) is the electric field, c is the light velocity in the free space, and ∈ is the permittivity of free space.

The time average power loss maps within solar cell are shown in Fig. 1(b) and Fig. 1(c). The incident wavelengths were 400 nm and 640 nm, respectively. It was calculated for an incident wave with an amplitude of 1 V/m. For the shorter wavelengths, most of the incoming lights are absorbed at the back of the solar cell in the C60 layer. This is due to the fact that the absorption coefficient of C60 material is very high in the shorter wavelengths of optical spectrum. The second maximum absorption of light is observed close to the interface of ZnPc:C60 and C60 layers due to the presence of C60 in the blend layer and a little contribution from the active material. Whereas, a comparatively higher absorption coefficient of absorber layer in the longer wavelengths, resulting the maximum absorption of incident light only in the active region for the monochromatic wavelength of 640 nm.

2.2 Toward an Optimal Flat Structure by Observing the Influence of Thickness

In order to obtain an optimal structure of flat solar cell that gives maximum short circuit current and quantum efficiency, the influence of each layer thickness on short circuit current and quantum efficiency was investigated. The quantum efficiency for an organic solar cell can be calculated as the ratio of the power absorbed in the organic absorber material to the total power incident (P_{Opt}) on the unit cell. The following equation (2) was used to calculate the quantum efficiency:

$$QE = \frac{1}{P_{Opt}} \int Q(x,y)\, dxdy \qquad (2)$$

Since the internal quantum efficiency for thin-film organic solar cells is assumed to be 100%, the results present an upper limit of the external quantum efficiency and short circuit current. The short circuit current was calculated based on the external quantum efficiency using the following equation (3):

$$I_{SC} = \frac{q}{hc} \int_{\lambda_{min}}^{\lambda_{max}} \lambda \,.\, QE(\lambda).\, S(\lambda) d\lambda \qquad (3)$$

where h is Planck’s constant, c is the light velocity, q is the elementary charge, λ is the wavelength, and S(λ) is the spectral irradiance of sunlight (AM 1.5).

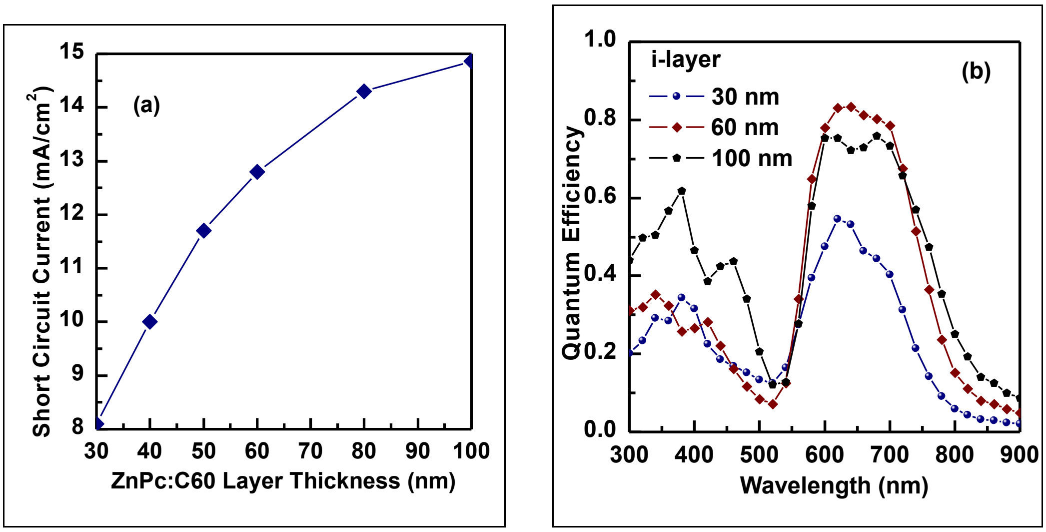

Fig. 2: a) Short circuit current as a function of ZnPc:C60 thickness for the cell. b) Comparison of quantum efficiency for n-i-p organic solar cell with the variation of ZnPc:C60 layer thickness.

The thickness of the ZnPc:C60 layer was varied from 30 nm to 100 nm as shown in Fig. 2, whereas thickness for other layers were kept constant. As the thickness of the absorbing layer of the solar cell is increased, a significant increase of the short circuit current as well as the quantum efficiency was observed. For an i-layer thickness of 100 nm, the short circuit current increases from 8.11 mA/cm^2 to 14.85 mA/cm^2. But, we cannot merely increase the thickness of the absorber since it might create additional defects in the band gap acting as recombination centers for photogenerated carriers, which in turn deteriorates its electrical properties. So we will consider 60 nm as an optimal thickness. The C60 layer was also varied for the short circuit current and quantum efficiency as shown in Fig. 3. Compared to the reference structure as depicted in Fig. 1(a), the cell with a 25 nm thickness of C60 layer was achieved a maximum of around 6.5% higher short circuit current from 12.81 mA/cm^2. Because of the high band-gap property of ITO, TiO2, and MeO-TPD, they are almost transparent for longer wavelengths of optical spectrum though a very few power loss is pronounced in the shorter wavelengths. So the influence of the variation of thickness on these transparent layers can be negligible for short circuit current and quantum efficiency. For the optical spacer property of TiO2 layer, it plays a major role for the optimization.

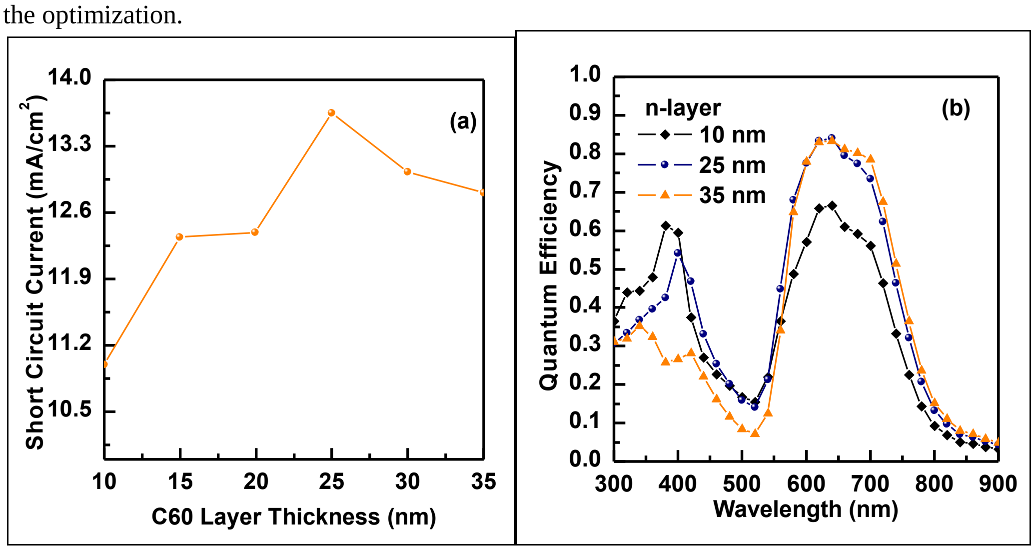

Fig. 3: a) Short circuit current as a function of C60 thickness for the cell. b) Comparison of quantum efficiency for n-i-p organic solar cell with the variation of C60 layer thickness.

A solar cell without spacer has relatively a large fraction of the absorber layer in a dead-zone in which most of the excitons are generated near the ITO/MeO-TPD electrode and consequently the photogeneration carriers are significantly reduced. The spacer tunes the position of the active region with respect to the light intensity of electric fields by varying the thickness in such a way that the maximum intensity of light get absorbed on the absorber layer [7]. In order to obtain an optimal thickness of the TiO2, the thickness of the

TiO2 layer was varied from 0 nm (no TiO2 layer) to 100 nm as depicted in Fig. 4. The maximum short circuit current of 12.81 mA/cm^2 was obtained with the introduction of a 10 nm TiO2 layer.

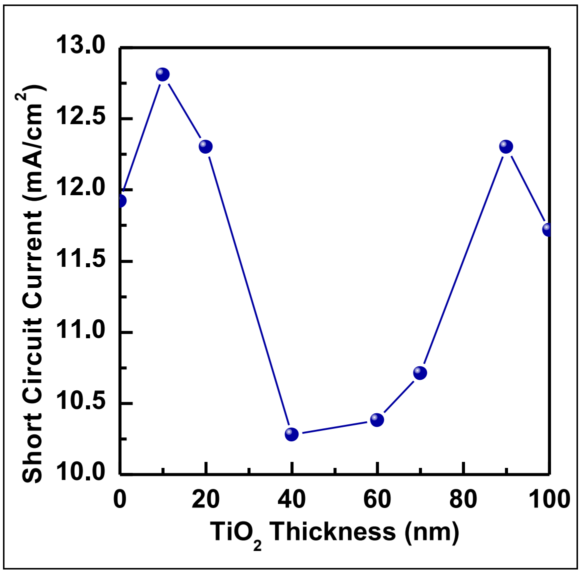

Fig. 4: Short circuit current as a function of TiO2 thickness for the cell.

2.3 Optimized Solar Cell for Smooth Substrate

Based on the best short circuit current and quantum efficiency, an optimal solar cell layer sequence, ITO(130 nm)/MeOTPD(20 nm)/ZnPc:C60(60 nm)/C60(25 nm)/TiO2 (10 nm), has been obtained. The optimal flat solar cell structure leads to an increase of the short circuit current by 0.84 mA/cm2, resulting in a short circuit current density of 13.65 mA/cm2. The quantum efficiency plot along with parasitic absorption losses of other layers for the optimized organic solar cell with smooth surface is depicted in Fig. 5.

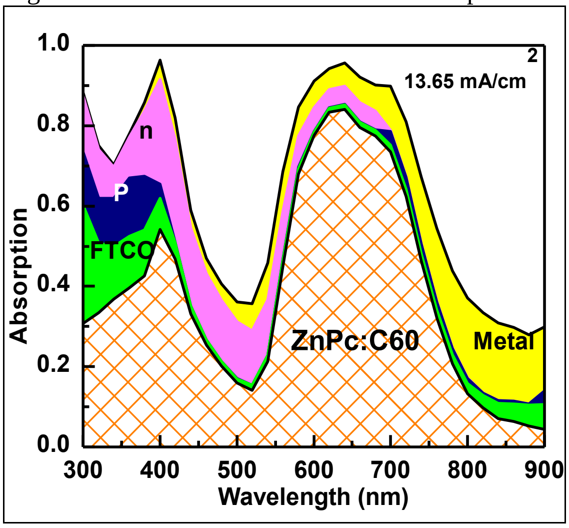

Fig. 5: Quantum efficiency and parasitic absorption plot for optimized substrate (n-i-p) organic solar cell with smooth surface.

The optimal structure exhibits an advantage of the quantum efficiency in the region 300 nm - 600 nm, since the structure was adjusted by obtaining the best thickness of C60 layer which has better absorption in that region. In terms of the parasitic absorptions, the ITO, TiO2, MeO-TPD, and Al metal layers absorb 1.11%, 2%, 0.16 %, and 5.74 %, respectively at 640 nm, whereas C60 absorbs almost 4.56% of the total absorbed light in the entire solar cell stack. The largest loss is observed for C60 layer mainly for the shorter wavelengths (300 – 500 nm), while the loss is on average almost less than 2% from 600 nm - 800 nm of optical spectral range. The absorption loss for ITO and MeO-TPD is mainly observed in the wavelength range of 300 - 420 nm, whereas it is almost transparent for the longer wavelengths. Optical loss in the Al layer increases for the longer wavelengths although it is very low for the shorter wavelengths. The absorption on the TiO_2 is quite negligible and has not been presented here. The information on the total reflection can also be extracted from Fig. 5. The reflection can be calculated as R = 1 − A, where A is the total absorption of the solar cell. It can be observed that for 400 - 600 nm and 700 - 900 nm of spectral range, the upper portion of the figure is white, representing the total reflection from the solar cell.

III. Modeling for light trapping pyramid textured surface

From the investigation of smooth substrate thin-film organic solar cell, it has been observed that the absorption in the solar cell is distinctly decreased for the shorter wavelengths. Reflections of 30.14%, 63.44%, and 3.92% were calculated for wavelengths of 340 nm, 520 nm, and 640 nm. Therefore, efficient light trapping concepts are needed to increase the effective thickness of the solar cell for shorter wavelengths. In this research project, a light trapping pyramid textured has been proposed, which can be applied to enhance the optical path length inside the cell for higher absorption in the photoactive layer.

3.1 Optical Simulation Model

Organic solar cells with textured contact layers can be realized by growing the solar cell directly on a textured back (n-i-p solar cell) contact. Textured and transparent contact layers can be fabricated by the direct growth of rutile titanium dioxide (TiO2) films via facile and one-pot hydrothermal method, which exhibits a pyramid-like texture [6]. The optical simulations can be carried out for 3-dimensional case, where the three dimensional surface texture is presented by arrays of square based pyramid structures that are periodic in both x- and y- direction. The wave propagation in the textured organic solar cells can be studied by simulating the optics in three dimensions. In this proposed model, a three dimensional surface coverage technique has been implemented to generate film morphology under the assumption that the organic film grows in the direction of the local surface normal by using the surface morphology of periodic textured substrate and film thickness as input data.

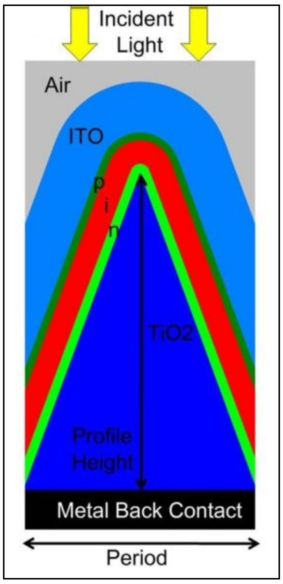

Fig. 6: Schematic sketch of the unit cell of a periodically textured thin-film substrate (n-i-p) organic solar cell for pyramid surface texture.

It makes the deposited film thickness equal for each position of the substrate i.e., each point of the substrate the surface coverage algorithm assumes an equidistant surface, which connects to the film surface predicted by substrate points for which the surface point is defined. It increases the effective thickness of the thin-film organic solar cells. A schematic cross section of a periodic pyramid textured substrate organic solar cell is shown in Fig. 6(a). The cross section of the pyramid textured solar cell is taken in the middle of the unit cell; therefore it resembles a triangle-like texture. The structure can be investigated by varying period, height, and in terms of the opening angle. The unit solar cell can be illuminated under normal incidence using a standard AM 1.5 sun spectrum. The input wave can be assumed to be circularly polarized for the simulations. The effective thickness of the organic pyramid textured solar cell can be calculated by the ratio of volume occupied by layers to the surface area. Since the 3-dimensional surface texture is presented by arrays of squared based pyramid structures which are periodic in both x- and y- direction, the effective thickness relation in terms of height of pyramid can be given as the equation (4):

$$Effective\ Thickness = \frac{\sum height(x,y)dxdy}{period \times period} \qquad (4)$$

As the pyramid height increases, the effective thickness of solar cell increases as well which can be seen from Fig. 7. Although the effective thickness of the flat solar cell (no height) for all of the periods converge to the actual thickness (60 nm) of the cell, a comparatively much more higher increase of effective thickness is observed with different heights for the period of 200 nm. This increased effective thickness of 200 nm of period and 1500 nm of pyramid height will result in the increased absorption and short circuit current due to the enhanced scattering and light trapping.

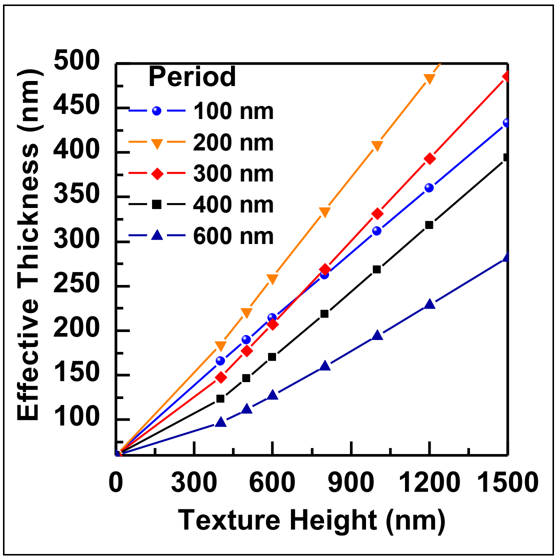

Fig. 7: A comparison of the effective thickness plot of the organic pyramid solar cell with different pyramid period and height.

IV. Conclusion

In this research, an optical modeling for efficient light trapping and incoupling of wave propagation in thin-film substrate configuration organic solar cells for pyramid surface texture was proposed. Introduction of pyramid texture increases the effective thickness, which can lead to create multiple bounces of an incident light ray and increase the optical path length. The maximum enhancement of effective thickness is observed for a pyramid period of about 200 nm and height of 1500 nm. The influence of thickness on short circuit current and quantum efficiency for n-i-p devices with photoactive layer system consisting of ZnPc:C60 blend of organic material was studied and an optimal substrate flat organic solar cells was obtained. The optimized flat solar cell achieves 13.65 mA/cm2 short circuit current with a maximum 84% quantum efficiency in 640 nm.

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