Nanohole Design for High Performance Polymer Solar Cell

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***Abstract* –A novel design of nanohole polymer solar cell (NHPSC) is reported for light trapping improvement. The proposed design has shown a considerable enhancement in the optical and electrical parameters of the polymer solar cell based on a conventional blend of poly-3-hexylthiophene/ [6, 6]-phenyl-C61-butyric acid methyl ester (P3HT:PCBM) as an active material. In this study, 3D finite difference time domain method is used to simulate the light absorption in the nanohole structure. In addition, an electrical model is developed to calculate the electrical parameters of the polymer solar cell. The reported design has shown 28% improvement in short circuit current density and overall efficiency alike.**

Index Terms – solar cell; nanohole; opto-electrical model

I. Introduction

In recent years, organic solar cells (SCs) have gained enormous interest due to their low cost, flexibility and large area [1]. However, the low efficiency of organic solar cells which around 5% [2-5] remains a massive challenge. As a result, a number of different techniques has been investigated to improve the efficiency of the organic solar cell such as; localized surface plasmon on metal nanoparticles [3, 4] and plasmonic cavity [5]. Currently, nanostructures have grown as the main building block to construct light-trapping which can improve the absorption in the active materials as well as the overall efficiency of the solar cell [6].The use of sub-wavelength nanostructure has gained a great attention due to its high ability of light trapping by increasing the optical bath length. Consequently, the photon absorption inside the active material can be enhanced [7]. Electrical modeling is one of the most important aspects for studying the performance of the solar cell and calculating the power conversion efficiency. Therefore, a number of studies has been reported to obtain the electrical parameters of the solar cell [2, 8].

In this paper, the optical and electrical properties for nanohole (NH) polymer solar cell, based on poly-3-hexylthiophene/ [6, 6]-phenyl-C61-butyric acid methyl ester (P3HT:PCBM) as an active material, have been investigated. The finite difference time domain method is used to obtain the optical properties of the suggested nanohole polymer solar cell (NHPSC) structure which shows a dramatic enhancement in the light absorption with a significant refinement in the short current density and overall efficiency. In addition, an electrical model based on single diode model and electron diffusion differential model [8] has been developed to calculate the electrical parameters and overall efficiency. The numerical results reveal that the proposed new design has the potential to improve the short circuit current and overall efficiency by around 28% compared to the conventional photonic crystal (PC) polymer SC [6]. To the best of our knowledge, this is the first time to introduce a complete opto-electrical model for polymer solar cell to study its optical and electrical properties and obtain the power conversion efficiency of the cell.

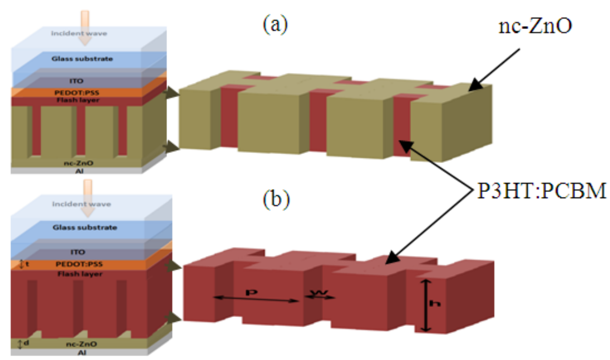

Fig. 1 Schematic diagram of polymer solar cell based on (a) conventional PC [6] and (b) proposed NH structure

II. Design considerations

The conventional polymer solar cell structure consists of glass substrate coated by anode layer of Indium tin oxide (ITO) and hole block layer of PEDOT:PSS as shown in Fig. 1 (a). In addition, P3HT:PCBM nanostructure photoactive layer is coated over the PEDOT:PSS layer. Moreover, a layer of nano crystalline Zinc oxide (nc-ZnO) is used as an electron transport layer. Finally a layer of aluminium (Al) is used as a cathode. It should be noted that, a flash flat layer of P3HT:PCBM is needed to prevent the direct contact between the PEDOT:PSS layer and the (nc-ZnO) layer [9]. In this investigation, our proposed design has a square NH lattice with periodicity (p) as shown in Fig. 1 (b). The NH with height (h) and width (w) is embedded into the photoactive layer P3HT: PCBM. The NH structure is periodic along x and y directions. Therefore, to save the simulation time, we simulate only one unit cell of the structure and the boundary conditions are taken as anti-symmetric along x-direction and symmetric along y-direction. In addition, perfect matching layers (PML) boundary conditions are used along z-direction. In this study, a plane wave is incident normally on the glass substrate where the reflection from the air-glass interface is overridden.

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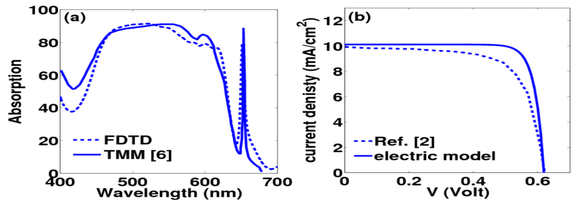

Fig. 2 (a) absorption of the conventional PC based SC calculated by TMM [6] and FDTD method. (b) J-V curve calculated by our model and model of Ref. [2]

III. Numerical Results

The 3D Finite Difference Time Domain Method (FDTD) is applied by using Lumerical FDTD Solutions package to simulate the light absorption in the NH structure. Our reported electrical model considers the polymer solar cell as a single diode and applies Green empirical expression for the fill factor to calculate its electrical parameters. Then by applying the electron diffusion differential model according to Ref. [8] we can find the internal parameters of the cell which help us to obtain the characteristic (J-V) curve of the polymer solar cell. In order to validate the opto-electrical model, Fig. 2 (a) shows a comparison between the absorption curves of the conventional PC based polymer SC calculated by two different methods, transvers matrix method (TMM) [6] and FDTD method. Fig. 2 (b) shows a comparison between our electrical model and the electrical model at Ref. [2]. It is revealed from Fig. 2 that there is a good agreement between our results and those in the literature [6, 2]. The suggested NHPSC is optimized as following; the thickness of the Aluminum layer (Al), ITO, nc-ZnO and PEDOT: PSS are fixed to 100nm, 178nm, 75nm, 50nm, respectively. In addition, the P3HT:PCBM flash layer thickness is equal to 40 nm. Moreover, the height (h) and width (w) of NH are taken as 300 nm and 205 nm, respectively. The short circuit current can be calculated through (1) by assuming that, every incident photon can produce electron which can successfully achieve the electrode and contribute to the photocurrent [10].

$$J_{SC} = \int I(\lambda)A(\lambda)e\lambda / hc \ \ \mathrm{d}\lambda \qquad (1)$$

where I (λ) is the spectral irradiance of standard air mass 1.5 (AM1.5), A (λ) is the optical absorption, e is the charge of electron, h is Planck's constant and c is the velocity of light.

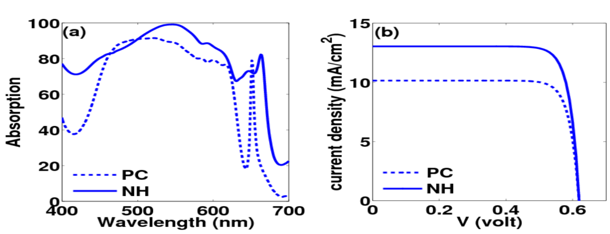

Fig. 3 (a) The optical absorption and (b) J-V curve for conventional PC and proposed NH based polymer solar cells.

The complex refractive index of the nc-ZnO and the active material (P3HT:PCBM) are following Ref. [6]. It should be noted that, the glass substrate, ITO, PEDOT:PSS and nc-ZnO are considered to be transparent [6]. Consequently, the reported absorption in Fig. 3 (a) represents the optical losses only in the active material. Fig. 3 (a) shows a considerable enhancement in the optical absorption of the proposed NHPSC compared to the absorption of the conventional PC polymer solar cell. This is due to the high contrast in refractive index between the nanohole and its surrounding active medium (P3HT: PCBM). Therefore, in-plane confinement has occurred due to the total internal reflection between the low refractive index of the nanohole and the high refractive index of the surrounding active material. The high confinement of the light inside the active material increases the optical path length which increases the chance for the photons to be absorbed in the photoactive material (P3HT: PCBM). In addition, the enhancement of the absorbed photons is directly contributed to photocurrent density improvement as shown in Fig. 3 (b).

In conclusion, table 1 shows a comparison between the calculated parameters of the conventional PC and our suggested NH based polymer solar cells.

Table 1: The electrical parameters of PC and NH based polymer solar cells.

Type	Jsc(mA/cm^2)	Efficiency	Voc(volt)
PC	10.13	5.032	0.62
NH	13	6.716	0.62
Improvement	28.7%	28.5%	

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