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Red and near-infrared absorption enhancement for low bandgap polymer solar cells by combining the optical microcavity and optical spacers

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ABSTRACT

Metal-mirror microcavity (MMC) structure is incorporated into the low bandgap polymer solar cells (LBPSCs) by sandwiching the active layer between the semitransparent Ag electrode and top Ag electrode. Optical simulations demonstrate that significant absorption enhancement can be achieved in the red and near infrared (near-IR) wavelength range due to the large optical electric field confined by the MMC structure. By inserting optical spacers to control the spectral and spatial distribution of the electric field in the LBPSC devices, the MMC structure can improve the total absorbed photons (TAPs) at the red and near-IR spectral range (620–900 nm) by 42.6% and yield an improvement of 14.0% in TAPs across the whole spectrum (400–900 nm) for the device with a 100 nm-thick active layer. For devices with thinner active layer, the improving rate is significantly raised to over 100%. Additionally, it is revealed that the effects of the optical spacers on the electric field distribution vary with their positions in the MMC structure. Finally, the MMC-based devices are optimized by tailoring the electric field distribution in the devices.

1. Introduction

Low bandgap polymer solar cells (LBPSCs) have attracted increasing attention in recent years due to their capability of converting the photons within the near-infrared (near-IR) part of the sun spectrum into electricity[1–7]. By reducing the bandgap of the polymers to harvest more sunlight and lowering the highest occupied molecular orbital of the polymers to increase the open-circuit voltage, the power conversion efficiency (PCE) of the devices have reached as high as 7.4% [1–2]. However, the device performance is still hindered by the low external quantum efficiency (EQE) within the near-IR wavelength range, which is mainly caused by the poor photon absorption in this wavelength range[1–7]. One of the factors preventing the near-IR photons from being well absorbed is that the active thickness layer is limited by the carrier recombination in the polymers [7]. Therefore, maximizing the near-IR absorption in the active layer with limited thickness is a critical issue towards enabling high-efficiency PSCs. Light trapping techniques such as surface Plasmon [8,9], optical spacer,[10–12] and metal-mirror microcavity (MMC) structure [13–17] have been developed to manage the photons inside the PSC devices and then increase the photon absorption in a specific wavelength range. The focus of these studies is on the management of the photons within visible wavelength range for the PSCs with high bandgap material as active layer [8–17]. But to date, little information has been provided in previous literature concerning the near-IR photon management for the LBPSCs [18].

Another issue regarding the PSCs is the role of optical spacers in the devices. It is well known that inserting an optical spacer between the active layer and the top metal electrode can redistribute the optical electric field spatially and shift the active layer into the maximum of the electric field [10–12]. Recently, it is claimed that the same purpose can be achieved by inserting an optical spacer between the active layer and semitransparent metal electrode of the MMC-based devices, which is constructed by sandwiching the active layer between two silver (Ag) mirrors [17]. A more recent study demonstrates that even the layer between the active layer and transparent indium tin oxide (ITO) electrode can affect the electric field distribution in the PSC device [5]. In fact, when inserted at different places in these devices, the optical spacers should play a different role since the devices consist of an asymmetrical structure with the active layer sandwiched between a semitransparent metal electrode/transparent ITO electrode and a highly reflective metal electrode. Yet, this point has not been clearly expatiated in previous studies so far.

The paper aims to develop light trapping technique based on the MMC structure to improve the red and near-IR photon absorption for LBPSCs and elaborate how the optical spacers control the electric field distribution in the MMC-based PSCs. For this purpose, transfer matrix method (TMM) [19–21] and optical

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interference theory are employed to investigate the optical performance of the MMC-based LBPSC devices. It is demonstrated that by controlling the electric field distribution in the MMC structure the total absorbed photons (TAPs) at the red and near-IR spectral range (620 nm–900 nm) can be improved by 42.6% for the device with a 100 nm-thick active layer. In addition the paper focuses on distinguishing the effects of the optical spacers on the spectral and spatial distribution of the electric field, when they are inserted at different places in the MMC-based LBPSCs. It is revealed that the effects of the optical spacers vary with their positions in the MMC structure. Finally, calculations are performed to optimize the optical performance for MMC-based devices by controlling the electric field distribution in the devices.

2. Device structure and theoretical model

2.1. Materials and device structure

As is shown in Fig. 1(a), the MMC-based LBPSCs used for simulation are assumed to have an inverted structure of capping layer/semitransparent Ag cathode /electron transport layer (ETL)/ active layer/hole transport layer (HTL) /Ag anode. In the devices, the active layer is assumed to be made from a blend of poly[2,6-(4,4-bis-(2-ethylhexyl)- 4H-cyclopenta[2,1-b;3,4-b′]dithiophene) -alt-4,7- (2,1,3-benzothiadiazole) (PCPDTBT) and 1-(3-methoxycarbonyl) propyl-1- phenyl(6,6)C61($PC_{60}BM$). The PCPDTBT has a low band gap of about 1.4 eV and light absorption in the active layer starts at a wavelength of about 900 nm [19], as shown in Fig. 1(b).

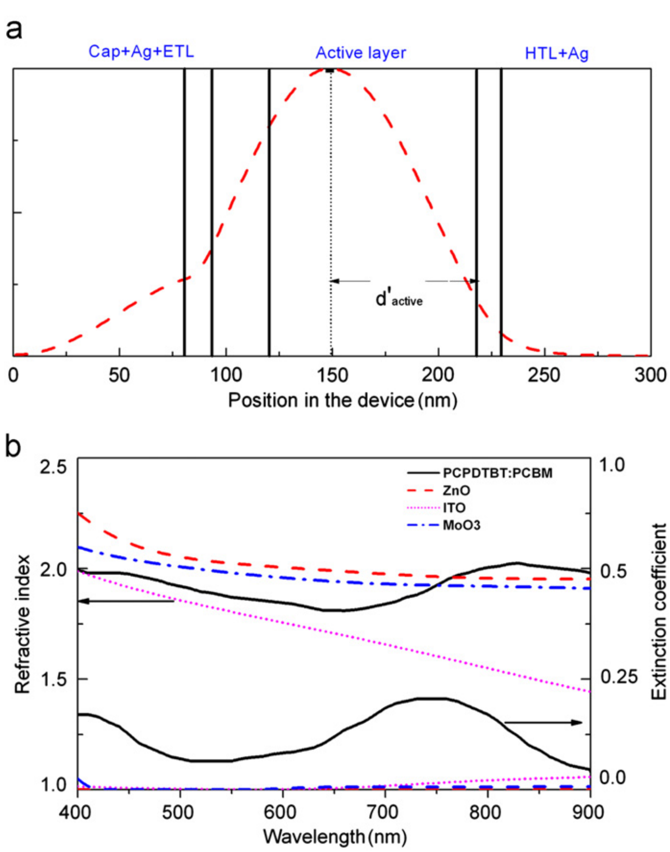

Fig. 1. (a) Structure of the MMC-based LBPSCs. The red dashed line denotes the normalized $|E(x)|^2$ for the light with the wavelength of 734 nm; d'_{active} is the distance between the first-order electric field antinode and the active layer/HTL interface. (b) Refraction index and extinction coefficient of PCPDTBT:PCBM, ITO, ZnO and MoO_3 used for the simulations. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

MoO_3 and ZnO layers are used as HTL and ETL, respectively, which meanwhile act as optical spacers [10–12,14,17]. For convenience, the HTL is referred to as optical spacer I and the ETL as optical spacer II. The semitransparent Ag cathode and top Ag anode act as the cavity mirrors for the MMC structure. A thin MoO_3 layer is capped on the semitransparent Ag cathode to increase light coupling and tailor the reflection of the cavity mirror.

2.2. Theoretical model

2.2.1. Optical modeling

Optical modeling based on transfer matrix method (TMM) is employed to calculate the optical absorption in the active layer. The model first calculates the optical electric field $E(x)$ at each position in the device using the TMM. Based on the calculated $E(x)$, the optical absorption in the active layer is described as a function of the real and imaginary parts of the refractive index of each layer [19–21]:

$$A(\lambda) = \frac{1}{I(\lambda)} \int_{x \in \text{layer}} \frac{2\pi c \varepsilon_0 k n |E(x)|^2}{\lambda} dx \tag{1}$$

where $I(\lambda)$ is the light intensity in the glass transferred to the glass/ITO interface, c is the speed of light, ε_0 is the permittivity of vacuum, λ is the vacuum wavelength, n and k denote the refraction index and extinction coefficient and $E(x)$ is the total optical electric field at point x.

With the absorption data obtained from Eq. (1) as input parameters, the total absorbed photons (TAPs) in the active layer are obtained by integrating the absorbed photons in the wavelength range from 400 nm to 900 nm. In the calculation, the devices are assumed to be illuminated with $AM_{1.5}$ at 100 mW/cm^2. All the complex refraction indices of the materials used for simulations is extracted from Refs. [22–26] and shown in Fig. 1(b).

2.2.2. Optical interference theory

Optical interference theory is employed to analyze the optical characteristics of the MMC-based LBPSCs. In this type of devices, the incident light makes round trip between the two cavity mirrors and optical resonance occurs at the resonance condition [27–28]:

$$\sum n_i d_i + L_{pen1} + L_{pen2} = m\lambda/2 \tag{2}$$

where n_i and d_i are refractive indices and thickness of the layers between the two Ag mirrors, L_{pen1} and L_{pen2} are the penetration depth of the semitransparent Ag mirror and thick Ag mirror, λ is the wavelength of the incident light, and m is the number of the cavity mode. The left term of the equation denotes the total optical length of the microcavity, and is named as $L(\lambda)$.

When Eq. (2) is met, namely, the ratio of cavity length to half-wavelength ($2L(\lambda)/\lambda$) equal to an integer number, the optical electric field in the MMC structure will be significantly enhanced due to the microcavity resonance effects. However, for the MMC-based devices with active layer much thinner than the wavelength of the incident light, the microcavity-enhanced electric field does not necessarily lead to absorption enhancement unless the spatial distribution of the electric field is optimized to position the electric field antinode in the active layer.

According to the optical interference theory, the position of the electric field antinode in the MMC structure can be expressed as [29]

$$\sum n_i d_i = \frac{m\lambda}{2} - \frac{\psi}{4\pi}\lambda \tag{3}$$

where the left term ($\Sigma n_i d_i$) denotes the optical distance between the electric field antinodes and the top Ag electrode, n_i and d_i are the refractive indices and thickness of the layers between the electric