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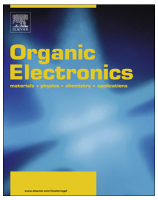

Predicting photocurrent tendency of organic photodiodes operating at external bias through optical field modeling

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ABSTRACT

Optical field distribution and electric field distribution in organic photodiodes (OPDs) are of great importance for exciton generation and photocurrent improvement. Therefore, the influence of the two factors on the properties of OPDs should be considered simultaneously to get optimal devices. In this research, we analyzed the dependence of the photocurrents of m-MTDATA/C_{60} heterojunction OPDs on the light absorption and electric field distribution. And then a model was set up for predicting the tendency of photocurrent changing with the thicknesses of devices. The validity of the model was well verified by the consistency of the simulated data and the experimental data. Devices built according to the simulated optimal configurations gained improved photocurrents as expected. Furthermore, based on the model, we also presented a simple method to estimate the diffusion length of C_{60}, which may be suitable for other materials.

1. Introduction

Photodiodes based on organic materials have attracted considerable attention due to their unique advantages, such as large-area low-cost fabrication, superior mechanical character, high sensitivity and the ability to select the wavelength of light absorbed [1–3]. For their abundant promising applications in signal processing, optical sensing system, and image sensor [4–7], it is significant for us to pursue a higher performance of organic photodiodes (OPDs). Several reports have focused on the performance improvement of OPDs [8–11]. The effects of morphology, temperature, light wavelength and work function on the device performance have been studied. However, few studies of dependence of photocurrents on optical field distribution and then on the thickness of the active layer in device were carried out. The intensity of the optical field in an OPD is considered to have wave-like spatial distribution because of the effects of reflection and interference (see Supplementary material, Fig. S1) [12,13], which allows us to improve the photocurrents of OPDs through enhancing the optical field intensity near the p–n interface. Several studies on organic solar cells (OSCs) have employed optical modeling to investigate dependence of short-circuit current on the structure or the thickness of the devices and then get optimization of short-circuit current [14–16]. However, OSC and OPD devices differ in terms of process integration and operating systems although they may have similar stacks. OPDs operate at an external bias whereas OSCs do not, thus changing the thickness of the active layer of OPDs influences the carrier drift velocity by changing the electric field distribution. That brings uncertainty and difficulty to the optimization of OPD devices.

Here, we report our attempts to optimize the OPD devices through optical modeling, simultaneously taking the applied bias into account. Our research is based on a p–n heterojunction with p-type 4,4′,4″-tris{N,-(3-methylphenyl)-N-phenylamino} triphenylamine (m-MTDATA,

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Fig. 1a) and n-type fullerene C_{60} (Fig. 1a). The devices based on m-MTDATA and C_{60} have good photosensitivity, which has previously been investigated in our group [6]. By relating the optical field distribution with photogenerated carrier density, and then relating the electric field distribution with the photocurrent, we deduced equations which can be used to predict the tendency of the photocurrent when changing the thickness of m-MTDATA or C_{60}. Through comparing the simulated curves with experimental photocurrent data, the equations were proved reasonable. Meanwhile, we can also extract the diffusion length of excitons in C_{60} through this experiment.

2. Material and methods

2.1. Device fabrication

As shown in Fig. 1b, a series of m-MTDATA/C_{60} OPD devices with different thickness of active layers were designed and fabricated as the following structure: ITO(142 nm)/PEDOT:PSS (40 nm)/m-MTDATA (x nm)/C_{60} (y nm)/Al (120 nm), with active area of $3 \times 3\ \text{mm}^2$. ITO was patterned on the glass substrate as the anode. Firstly, a 40 nm PEDOT:PSS (CH8000, from H.C. Starck Clevios GmbH) layer was spin-coated onto an ITO substrate to smooth the ITO surface and improve the uniform of OPD performance, then the organic layers m-MTDATA (Sigma–Aldrich, used as received) and C_{60} (Nichem, used as received) were deposited by turns at a rate of 0.5 Å/s by thermal evaporation. Finally, Al cathode was deposited at 10 Å/s with the thickness of 120 nm. The degree of vacuum was controlled at 8×10^{-4} Pa when deposited and the deposition rates and thickness of the layers were monitored by oscillating quartz monitors. And the thicknesses of films were obtained by measuring the height difference between the film surface and substrate surface through Atomic Force Microscope method.

2.2. Characterization and testing

The photocurrents of OPD were measured by Keithley 4200 Semiconducting System. The EL spectrum of OLED was achieved by PR705 Photo Research Spectrophotometer. The optical constants, including refraction and extinction coefficient, were measured by SENTECH 850 Ellipsometer. The transmission of the thin film devices was measured by HATACHI U-3010 UV–Vis Spectrophotometer.

3. Theory and calculation

Our modeling process begins with the calculations of wave-like optical field distribution $E_p(x)$ (Fig. 1c) in the designed devices through transfer matrix method (TMM) (the details of this method were shown in the Supporting Information) [12,13], and then the total exciton generation rate (G) within the diffusion range of the p–n interface. Here we only took G into consideration because only the excitons generated within a diffusion range from the p–n interface, where they are expected dissociate, will contribute to the photocurrent [12,17,18]. Then we tried to relate the tendency of photocurrent and G under the consideration of electric field distribution.

4. Results and discussion

For the calculation of $E_p(x)$ through TMM, the typical optical constants of all layers in the OPD devices were measured by an ellipsometer. The measured index of refraction (n) and extinction coefficient (k) of m-MTDATA and C_{60} were shown in Fig. 2. $E_p(x)$ was deduced through solving the Eqs. (S1) to (S5) in the Supplementary material, To prove the reliability of the model and the optical parameters employed in our calculation, We compared the experimentally measured with the calculated

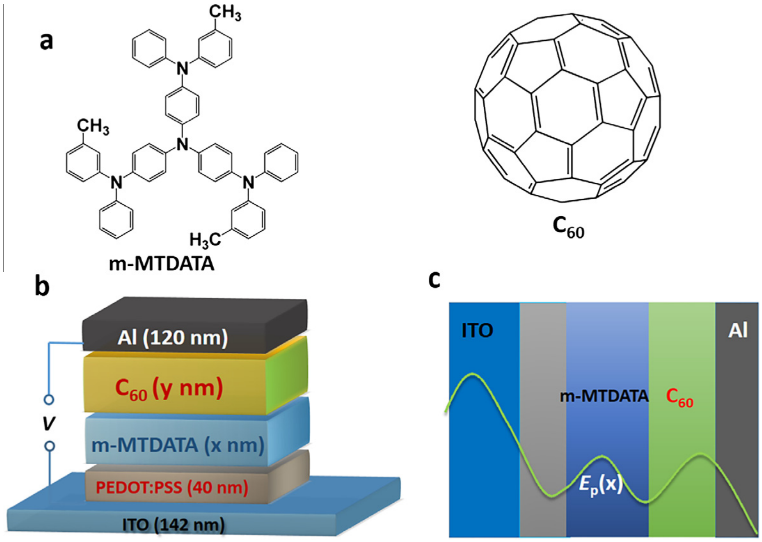

Fig. 1. (a) The molecular structure of m-MTDATA and C60. (b) Schematic of OPD device with m-MTDATA/C60-based heterojunction. (c) The wave-like spatial distribution of intensity of the optical electric field in organic photodiodes.