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Solar Energy Materials & Solar Cells

journal homepage: www.elsevier.com/locate/solmat

The effect of a buffer layer on the performance and optimal encapsulation time of ITO/CuPc/C₆₀/buffer/Cu bilayer cells

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ARTICLE INFO

Article history:

Received 7 July 2011

Received in revised form

4 September 2011

Accepted 5 September 2011

Available online 22 October 2011

Keywords:

Organic solar cells

Stability

Encapsulation time

YF₃C₆₀

CuPc

ABSTRACT

In this study, optical simulations have been performed based on a transfer matrix method (TMM) to investigate the performance of organic solar cells (OSCs). Then, the organic solar cells of configuration ITO/PEDOT:PSS/CuPc/C₆₀/EBL/Cu (Indium Tin Oxide/poly (3,4-ethylenedioxythiophene) polystyrene sulfonic acid/fullerene/Copper phthalocyanine/Exciton Blocking Layer(EBL)/Copper) were investigated. It is found that the performance of the cells gets slightly enhanced during the first 25 min after fabrication, and gradually declines afterwards. Therefore, all cells were removed from the vacuum after 25 min and encapsulated by YF₃. Then, the influence of a buffer layer such as lithium fluoride (LiF), bathocuproine (BCP), 4,7-diphenyl-1,10-phenanthroline (Bphen), tris-8-hydroxy-quinolinato aluminium (Alq₃) and CuPc was studied on the performance of OSCs. The highest efficiency was obtained for the devices with BCP or Bphen as their buffer layer. In particular, a half-lifetime of 90 days in air at ambient circumstance was achieved for LiF and CuPc as buffer layers.

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1. Introduction

Due to their flexibility, low-cost and light-weight organic solar cells (OSCs) devices have received considerable attention because of their potential advantages over their inorganic counterparts [1–5]. Power conversion efficiency and stability are the important parameters of organic solar cells for practical applications.

Some studies on the degradation of organic solar cells have focused on the oxidative damage to the active layers [6–9], physical degradation mechanisms [10], and illumination time [11].

Absorption of incident radiation by an individual layer depends on the optical constants and the thickness of the layer. Thus, copper phthalocyanine (CuPC) as a donor and fullerene (C₆₀) as an acceptor are commonly used structures based on small molecule organic solar cells. Inserting buffer layers or interface layers such as lithium fluoride (LiF), bathocuproine (BCP), 4,7-diphenyl-1,10-phenanthroline (Bphen), copper phthalocyanine (CuPc), 1,3,5-tris (2-N-phenylbenzimidazolyl) benzene (TPBI) and tris-8-hydroxy-quinolinato aluminium (Alq₃) between C₆₀ and the metal electrode has led to the improvement of the performance of OSCs [12,13]. The buffer layer generally prevents lowering of the work function of the C₆₀/cathode interface and blocks the diffusion of cathode atoms into the underlying organic layers during the deposition process [12–14].

Moreover, adequate encapsulation because of ambient oxygen and water is an essential requirement for the commercial viability of OSCs. The encapsulating layer, in turn, should be thin, defect-free, light-weighted, and easy to process. Various methods are reported in the literature, such as depositing an ultra thin barrier layer of Al₂O₃, lithium fluoride or MgF₂ between the active layer and the electrode, or top electrode [15–17].

The choice of electrode material is also critical to cell performance, and in many cases, determines the photovoltage as well as the photocurrent [18]. Silver [12], aluminium [19,20], gold [21], Ca/Al, WO₃/Al [22], and Yb [23] have been used as a contact in CuPc/C₆₀ organic solar cells in the past.

In this research, by using an optical modelling based on the transfer matrix method (TMM), the transmission, reflection, absorption, energy dissipation, and exciton generation rate in the structure of glass/ITO/PEDOT:PSS/CuPc/C₆₀/EBL/metal (Ag, Al and Cu) were investigated. Also, the degradation of solar device structures of ITO/PEDOT:PSS/C₆₀/CuPc/EBL/Cu/YF₃ with different buffer layers (such as: Bphen, Alq₃, CuPc, BCP and LiF) was studied. Then, the influence of the buffer layers on the current density–voltage (*J*–*V*) characteristics of OSCs was studied in detail. In addition, the role of a copper cathode and a protective layer in preventing oxygen and permeation through the organic layers was inquired.

2. Experimental

The configuration of the organic solar cells was ITO/PEDOT:PSS/CuPc/C₆₀/buffer/Cu/YF₃, where the buffer layers were either Bphen,

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Alq₃, CuPc, BCP or LiF. All the organic materials were purchased from Sigma-Aldrich. They had a high purity of 99%. An indium tin oxide (ITO)-coated glass substrate from Sigma-Aldrich with a sheet resistance of 15 Ω/sq was used as an anode, part of which was etched before cleaning with an area of approximately 0.7 × 0.5 cm². Then, ITO was cleaned sequentially in an ultrasonic bath containing detergent, propanol, acetone, and deionized water, and finally dried by high-purity nitrogen blow. Then the samples were spin coated with a thin layer of the conducting polymer poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) and were then dried in air at 120°C for 15 min. The organic materials were deposited onto the substrates successively by thermal evaporation at a rate of 0.1–0.2 nm s⁻¹ and a pressure of 6 × 10⁻⁴ Pa, followed by the deposition of Cu cathode at a rate of 0.2 nm s⁻¹ in VAS vacuum coating system. The deposition rate and the film thickness were monitored using a quartz crystal oscillator. The area of OSC cells was 0.3 × 0.5 = 0.15 cm². The current density–voltage (*J*–*V*) characteristics were measured for each cell with a Keithley 2400 source meter under an illumination of 100 mW/cm² with an AM1.5 G sun simulator.

3. Theory and simulation

A one-dimensional transfer matrix method [24] was used to simulate the optical field distribution within the device. The optical electric field in an arbitrary position inside the layer, *j*, is given in terms of the electric field of the incident wave (**E**₀) as follows:

$$\mathbf{E}_j(z) = \mathbf{E}_j^+(z) + \mathbf{E}_j^-(z) = (t_j^+ e^{i\epsilon_j z} + t_j^- e^{-i\epsilon_j z}) \mathbf{E}_0^+ \quad (1)$$

where $\epsilon_j = 2\pi(n_j + ik_j)/\lambda$, and n_j and k_j are optical index and extinction coefficient respectively. Also, t_j^+ and t_j^- are the electric fields propagating in positive and negative directions respectively. The local dissipated energy, $Q(z, \lambda)$, in the material at the depth point *z* for the wavelength λ in Wm⁻² nm⁻¹ can be obtained as [24]

$$Q(z, \lambda) = \frac{4\pi nk}{n_0 \lambda} I_{\text{solarlight}} \left| \frac{\mathbf{E}(z, \lambda)}{\mathbf{E}_0} \right|^2 \quad (2)$$

where n and n_0 are the real part of the complex refractive index of the layer and of the substrate, respectively, \mathbf{E}_0 is the amplitude of the incident electric field, and $I_{\text{solarlight}}$ is the polychromatic incoming light with a standard AM1.5 distribution (100 mW cm⁻²). The number of photons dissipated per second was calculated by dividing the dissipated energy $Q(z, \lambda)$ by the incoming photon energy. Then, the sum on all wavelengths in the visible spectrum was included, and we obtained the photon generation rate at the depth *z* as follows:

$$G(z) = \frac{1}{hc} \int_{300}^{900} Q(z, \lambda) \lambda d\lambda \quad (3)$$

Therefore, by assuming the exciton dissociation rate into charge carriers to be unity, the rate of exciton generation equals the carrier generation rate.

The optical performance of the design is calculated according to the characteristic matrix theory [25]. Provided that the incidence medium and the emission medium of this system are a half-infinite non-absorption mediums, its characteristic matrix can be formulated as follows:

$$\begin{pmatrix} B \\ C \end{pmatrix} = \left[\prod_{r=1}^k \begin{pmatrix} \cos \delta_r & \frac{i \sin \delta_r}{\eta_r} \\ i\eta_r \cos \delta_r & \cos \delta_r \end{pmatrix} \right] \begin{pmatrix} 1 \\ \eta_{k+1} \end{pmatrix} \quad (4)$$

where *B* and *C* are the electric and magnetic fields across the boundary respectively. η_{k+1} is the substrate admittance and δ_r is

the phase thickness which is defined as:

$$\delta_r = \frac{2\pi}{\lambda} N_r d_r \cos \theta_r = \frac{2\pi}{\lambda} (n_r - ik_r) d_r \cos \theta_r \quad (5)$$

In Eq. (5), d_r is the thickness of the medium. When the electric field is perpendicular to the plane of incidence, the parameter η_r is defined as follows:

$$\eta_r = N_r \cos \theta_r = (n_r - ik_r) \cos \theta_r \quad (6)$$

and for the parallel case, the parameter η_p is defined as

$$\eta_p = \frac{N_r}{\cos \theta_r} = \frac{(n_r - ik_r)}{\cos \theta_r} \quad (7)$$

Thus, the transmission, reflection and absorption of the general multilayer film system are calculated as

$$T = \frac{4\eta_0 \text{Re}(\eta_{k+1})}{(\eta_0 B + C)(\eta_0 B + C)^*} \quad (8)$$

$$R = \left(\frac{\eta_0 B - C}{\eta_0 B + C} \right) \left(\frac{\eta_0 B - C}{\eta_0 B + C} \right)^* \quad (9)$$

$$A = \frac{4\eta_0 \text{Re}(BC^* - \eta_{k+1})}{(\eta_0 B + C)(\eta_0 B + C)^*} \quad (10)$$

4. Results and discussion

4.1. Photovoltaic cell structure

The organic solar cell of interest is shown in Fig. 1a. Six layers deposited on top of the ITO layer which is deposited on a glass substrate: a PEDOT:PSS film, a donor layer CuPc, an acceptor layer C₆₀, a buffer layer or exciton blocking layer (EBL) (such as Bphen, Alq₃, CuPc, BCP and LiF) and a copper layer as a cathode.

The best performance of CuPc–C₆₀-based single bilayer hetero-junction cell has been reported for the device with the thickness of 20 nm and 40 nm for CuPc and C₆₀ respectively [26]. This optimization is based on the interference effect enhancing the optical field around the CuPc–C₆₀ active interface for exciton dissociation and the role of exciton diffusion length inside the layers.

Therefore, the thickness of each layer in the device was considered as: glass(1 mm)/ITO (120 nm)/PEDOT:PSS(50 nm)/CuPc (20 nm)/C₆₀(40 nm)/EBL(7 nm)/Cu(100 nm)/YF₃ (> 300 nm). Also, the thickness for LiF buffer layer was 1 nm. The role of a Yttrium (III) fluoride layer is to prevent oxygen and water from permeating through the organic layers and also to prevent the oxidation of the copper layer over time.

4.2. Optical constant

The optical constants (*n* and *k*) of each layer (organic or inorganic), which were used for optical simulation, were taken from several sources [27–29]. The refractive index (*n*) and the extinction coefficient (*k*) of each layer in the wavelength region from 300 nm to 800 nm for organic and inorganic layers are plotted in Figs. 2 and 3 respectively.

4.3. Simulation results

The optical model for the organic solar cell structures in this study is based on the transfer matrix formalism. The inputs to the model are the thickness and the complex refractive index (*n* and *k*) of each layer. The mathcad 14 software was used in all the calculations. The parameters which can be calculated from the output of the program include: relative electric field intensity,

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