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Original research article

Analytical modelling of organic solar cells with scattering interface

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ABSTRACT

Significant improvement of absorbance of regularly used Al/ZnO/poly (3-hexylthiophene) (P3HT): [6-6]-phenyl C_{61} butyric acid methyl ester (PCBM)/ poly(3,4-ethylenedioxythiophene) PEDOT/ Indium Tin Oxide (ITO) organic solar cell is achieved by inserting a scattering interface between ITO and PEDOT. The introduction of volumetric scattering mechanisms enhances the range of the absorbance spectrum and the absorbance of 100 nm active layer by 15%. There is an improvement of energy fluxby 34% at the centre of the spectrum and the generation rate increases roughly by 16% in the 450–750 nm window. The devices achieve a power conversion efficiency (PCE) of over 3.26% and an excellent external quantum efficiency (EQE) of 76.76%. The thick active layer in the device attenuates incident light almost completely without degrading the fill factor(FF) (69.6%–75.8%) and exhibiting a high short-circuit current density of 7.035 mA cm^{-2}.

1. Introduction

The demand foreconomical renewable energy source is the main motivation behind new approaches in the development of low cost solar photovoltaic devices [1–4]. Polymer solar cells offer enormous technological potential as a renewable and alternative source of electrical energy. Polymers, being economical light-weight materials, provide advantages of scalable fabrication and flexible substrates by on sale roll-to-roll techniques. For the past two decades, immense efforts have been made into the development of solar cells based on conjugated polymers with wide range of absorption and organic molecules [5–10]. Effective photon absorption controlPCE [2,11,12] in such polymers can be enhanced by light trapping mechanism [13,14] over anextensive range of wavelength.Conventional P3HT: PCBM organic solar cells have a structure of glass substrate/anode/hole transport layer (HTL)/active layer/electron transport layer (ETL)/cathode, where P3HT acts as an electron donor and PCBM acts as an electron acceptor layer [15–19].Internal quantum efficiency (IQE) which refers to the fraction of absorbed photons contributing to the generated photocurrent, can be tuned by varying the active layer thickness. Conjugate polymer solar cells, however suffers from a serious disadvantage of lower IQE due to the smaller thickness of the active layer in comparison to the absorption length. Increasing the active layer thickness to compensate IQE would severelyretard the hole mobility. Organic solar cells also undergo difficulties in charge transport which leads to poorer fill factor, recombination loss, and higher series resistance [20,21].

In this paper, we have proposed a solar cell structure followed by mathematical modelling of its absorbed scattering mechanism andoptical modelling (incoherent and scattering interface) of the simulated solar cell.The conversion efficiency, short circuit current density J_{SC} and open circuit voltage V_{OC} are investigated for the proposed device structure as the function of different parameters (i.e., wavelength, active layer thickness and angle of the incident light) by using acommercially available simulation software.

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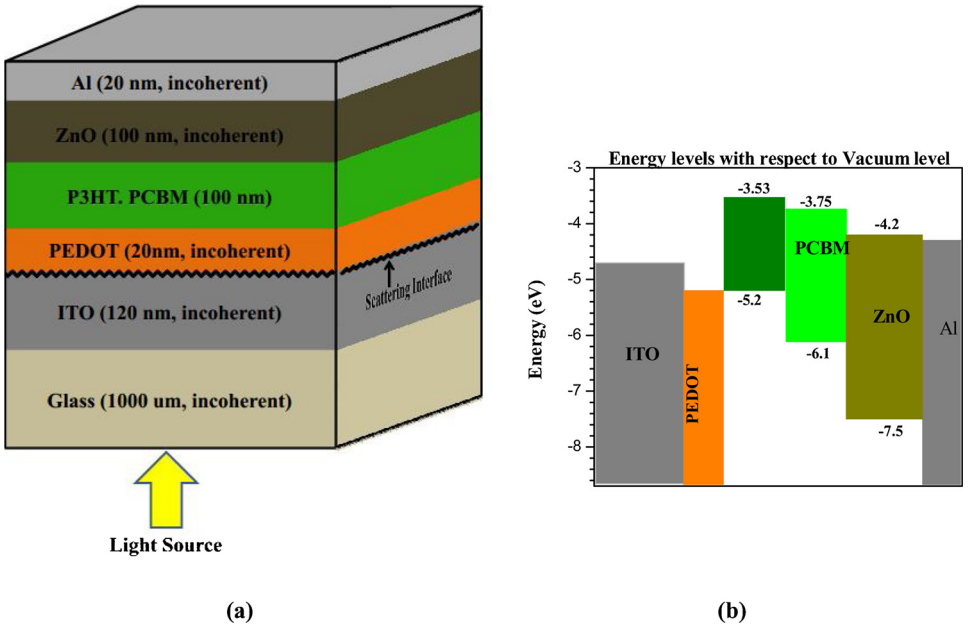

Fig. 1. (a) Schematic layer design of P3HT-PCBM (active layer) based solar cell with scattering interface and (b) The corresponding energy levels of different layers with respect to vacuum layer.

2. Proposed device structure

The solar cell structure is schematically shown in Fig. 1(a), where we have considered 1 mm incoherent glass with a high optical transmission of $>$ 85% and a low resistance of $<$ 10 O/sq. [22–27] as a substrate which is considered to have no phase correlation between the illuminated and the transmitted light. This is followed by an incoherent transparent electrode ITO of 120 nm thickness and 20 nm thick PEDOT layer, which is doped to allow conductivities of more than 500 S/cm and a transmission of $>$ 80% [28]. Ascattering interface with phong factor 49.1 and Haze 0.9 is inserted between ITO and PEDOT.The bulk heterojunction structure [29] of the active layer has a low carrier mobility and high absorption coefficient. Finally, the 100 nm ZnO layer used as an optical spacer helps to improve more photocurrent [30] and the 20 nm Al electrode collect the photo-generated electrons. Corresponding energy levels [31,32] of different layers with respect to the vacuum level is shown in Fig. 1(b). Active layer absorbs photons with energies between 1.65 eV and 2.34 eV and the conduction and valence band offsets of 0.22 eV and 0.9eVrespectively help to accelerate the electron and holes respectively.

3. Mathematical modelling

3.1. Volumetric scattering model

In this model, we have considered the intensity of the light only for the incoherent layers, which are thicker than the coherence length of the incident light and therefore do not allow coherent transmission of light. We have applied the scalar scattering theory [33] for our proposed scattering interface which exhibits volumetric scattering mechanism and is tuned by two important parameters- the Phong factor and Haze.The Phong factor and Haze define the scattered energy and specular angle for scattering respectively.Phong [34] proposed an analytical model for the angular distribution function, $I(\theta)$ of the diffusely scattered portion of the light is

$$I(\theta) = C\cos^{l}(\theta - \theta_{spec}) \tag{1}$$

whereC is normalization constant, l is the phong exponent and θ_{spec} is the direction ofspecular reflection or transmission. The Phong factor usually lies between 1 and 100 though higher values of Phong factor leads to more specular light. Specular light spectrum leads to creation of more excitons in the photoactive layer due to the increase in scattered energy. There is a tradeoff between phong factor and θ_{spec}.We have taken the optimized values of Phong factor (49.1) and the angular range (0–3°)to achieve the best possible outcome.

The Haze parameter for rough interface can be defined as

$$H_T = 1 - \exp\left[-\left(\frac{4\pi\sigma_{rms}c(\lambda)|n_1\cos(\phi_{inc}) - n_2\cos(\phi_t)|}{\lambda}\right)^3\right] \tag{2}$$

where $c(\lambda)$ represents a correction function for the projection of light scattering at internal interfaces [35], σ_{rms} is the root-mean-