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3D full-wave optical and electronic modeling of organic bulk-heterojunction solar cells: a predictive approach

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ABSTRACT

A predictive approach using 3D full-wave optical and electronic modeling of an organic bulk-heterojunction photovoltaic device (P3HT:PCBM) is presented. The optical part is modeled by solving 3D frequency domain Maxwells equations such that the scattering of subwavelength nanostructures can be modeled accurately. The electronic simulation which consists of solving the rate equations to account for the generation and recombination of polarons or charges, and the flow of electrons and holes are assumed to be drift-diffusion in nature. Here, nanoparticles with subwavelength sizes are added to the P3HT:PCBM photovoltaic device and the current-voltage behavior is predicted by the model.

Keywords: Optoelectronic Model, Organic Semiconductor, Photovoltaic Cell

1. INTRODUCTION

The optoelectronic simulation of organic bulk-heterojunction (BHJ) photovoltaic devices typically consist of three parts: (i) optical absorption, where incident light is being absorbed by the active layer, (ii) polaron generation and recombination, where the energy of the photons absorbed does not generate electrons and holes straight away, but bounded electron-hole pairs (i.e. polaron pair) are generated and similarly free carriers can also recombine to form polaron pairs too, (iii) charge transport, where the dissociated free carriers from polaron pairs moved towards the electrodes under the influence of a built-in field and external bias.

Recently, a three-dimensional optoelectronic model is able to consider all the three important device physics as mentioned above.¹ However, in terms of polaron recombination a reduced form of the germinate recombination mechanism is being considered for a typical well-studied organic P3HT:PCBM bulk-heterojunction photovoltaic device. Therefore, the applicability of the model to a wide variety of different organic bulk-heterojunction solar cells, where the reduced germinate recombination mechanism may not be suitable, will be limited. Therefore, in order to improve the device model further, nongeminate recombination due to the interaction of free and trapped carriers must be included in the model. Furthermore, both external series (R_s) resistance must also taken into account in the calculation of the current density-voltage (J-V) characteristics of the organic solar cell.

In this manuscript, an improved 3D optoelectronic model, which can be applied to a wider variety of organic BHJ photovoltaic devices, will be demonstrated. The optical physics and equations which can also be found in Ref.¹ will be briefly reviewed in Sec. 2.1. The polaron and charge generation and recombination mechanisms with some modifications will also be discussed and shown in Sec. 2.2. Then, we apply the drift-diffusion charge transport and illustrate the corresponding boundary conditions for completeness in Sec. 2.3. In Sec. 3, we calibrate our 3D optoelectronic device model with experimental inputs for the control P3HT:PCBM organic solar cell make use of the calibrated results to predict the effect of the addition of Ag nanoellipsoids into the P3HT:PCBM organic photovotltaic (OPV) device.

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2. OPTOELECTRONIC MODEL

Our control model organic BHJ device structure consists of Glass(semi-infinite)/ ITO(130nm)/ PEDOT:PSS (45nm)/ P3HT:PCBM_{C₆₁}(200nm)/ Ca(10nm)/ Ag(100nm) where glass is the substrate, indium-tin-oxide (ITO) is the transparent cathode and silver (Ag) is the reflecting anode, 45nm thick poly (3,4-ethylenedioxythiophene) poly (styrenesulfonate) (PEDOT:PSS) is the transparent hole transporting layer, calcium (Ca) is the electron transporting layer, and last but not least poly(3-hexylthiophene) (P3HT) is the donor and phenyl-C₆₁-butyric acid methyl ester (PCBM) is the acceptor in the organic bulk heterojunction active layer. Typically, the thickness of glass in experimental devices is usually much greater than the thickness of the other layers. Thus, we can treat the glass substrate as a semi-infinite layer in the model. The permittivity of the materials used in the simulations can be obtained from.¹

2.1 Optical Modeling

Three-dimensional frequency domain Maxwell's equations are solved using the finite element method with normally incident monochromatic plane waves

$$\begin{aligned}\nabla \times \vec{H}_{opt} &= j2\pi\nu\epsilon_r\epsilon_0\vec{E}_{opt}, \\ \nabla \times \vec{E}_{opt} &= -j2\pi\nu\mu_0\vec{H}_{opt},\end{aligned}\quad (1)$$

where $\vec{H}_{opt}$ and $\vec{E}_{opt}$ are the optical magnetic and electric field vectors, ν is the frequency of the monochromatic wave, μ_0 , ϵ_0 are the permeability and permittivity of free space, $\epsilon_r = \epsilon_1 - j\epsilon_2$ is the frequency dependent relative dielectric permittivity of the material used in the OPV device.

Ports are placed at the top and bottom of the control cell to ensure that there are no reflected wave at the top and bottom boundaries. This is to simulate the semi-infinite glass substrate and semi-infinite region of air at the back of the Ag back reflector. As for the lateral boundaries, periodic boundary conditions are applied to the x and y boundaries of the cell. An input power of 1W is injected from the glass side of the cell and the magnitude of the energy density absorbed at each position (x, y, z) is later scaled with respect to the spectrum of interest (i.e. the AM1.5G solar spectrum).

The distribution of the total optical electric field $\vec{E}_{opt}(\nu, x, y, z)$ in the structure at each wave frequency ν is obtained from the solution of the 3D Maxwell's equations. We can then compute the spectral absorbed power density in the photoactive layer (P3HT:PCBM) at position (x, y, z) and at each frequency ν with

$$Q(\nu, x, y, z) = \pi\nu\epsilon_0\epsilon_2|E_{opt}(\nu, x, y, z)|^2, \quad (2)$$

where $-\epsilon_2 = Im(\epsilon_r)$ refers to the imaginary part of ϵ_r of P3HT:PCBM.²

2.2 Polaron Pairs & Charge Generation/Recombination

The total generation rate of polarons at each position of the bulk heterojunction is given as

$$G_{tot}(x, y, z) = \int_{AM1.5G} G(\nu, x, y, z)S(\nu)T_N(\nu)d\nu, \quad (3)$$

where $G(\nu, x, y, z) = \frac{Q}{h\nu} = \frac{\pi\epsilon_2\epsilon_0}{h}|E_{opt}|^2$ is the generation of polarons at each frequency ν and position (x, y, z) , where h is Planck's constant, $S(\nu)$ is the irradiance of the AM1.5G solar spectrum and $T_N(\nu)=0.961$ is the transmittance of glass (i.e. reflection at the air/glass interface is 3.9%).

The net generation and recombination of free carriers at steady state can be described by

$$k_{diss}X - R = G_{tot} - k_fX, \quad (4)$$

where $k_{diss}X - R$ is the net free carriers dissociated from the polarons, X is the polaron concentration at the position (x, y, z) , $k_f(x, y, z)$ is the non-radiative monomolecular recombination rate constant. The key equations describing the respective position dependent polaron dissociation, electron and hole bimolecular recombination rate constants (k_{diss} , R_n and R_p) and the probability of dissociation of polarons to free charges are given below:

$$\begin{aligned} k_{diss} &= \frac{3\gamma}{4\pi a^3} e^{-\frac{E_b}{k_B T}} \frac{J_1(2\sqrt{-2b})}{\sqrt{-2b}}, \\ R_n &= \gamma(n_f p_t - n_i p_i), \\ R_p &= \gamma(n_t p_f - n_i p_i), \end{aligned} \quad (5)$$

where $E_B = q^2/(4\pi\epsilon_{r0}\epsilon_0 a)$ is the polaron binding energy (based on the ion-pair model),³ q is the electronic charge, k_B is the Boltzmann constant, ϵ_{r0} is the effective static relative dielectric permittivity of the P3HT:PCBM blend, $b = q^3 E/(8\pi\epsilon_0\epsilon_{r0}k_B^2 T^2)$,⁴⁻⁷ E is the electrostatic field present in the active region, T is the temperature (taken to be 300K throughout the manuscript), $J_1(z)$ is the Bessel function of order 1, $\gamma = q(\mu_n + \mu_p)/(2\epsilon_0\epsilon_{r0})$ is the Langevin factor,⁵ $\mu_{n(p)}$ is the mobility of electrons (holes), n_f (p_f) is the free electron (hole) concentration, n_t (p_t) is the trapped electron (hole) concentration, $n_i = N_{LUMO} \exp\left(-\frac{E_{gap}}{2k_B T}\right)$ and $p_i = P_{HOMO} \exp\left(-\frac{E_{gap}}{2k_B T}\right)$ are the intrinsic electron and hole concentration, respectively. For n_i and p_i , N_{LUMO} and P_{HOMO} are the effective electron and hole density of states of the donor and acceptor respectively, and E_{gap} is the effective electronic bandgap of the blend, i.e. LUMO(PCBM)-HOMO(P3HT) [eV]. It is noted the mathematical form given for n_i and p_i has an implicit assumption that the Fermi level of the polymer blend is in the middle of the bandgap.

Instead of the reduced Langevin recombination factor used by Koh *et al*, we adopt the description of the trapped carriers⁸ to account for the reduced recombination as several recent studies have identified that the recombination mechanism for polythiophenes are nongeminate in nature and charge density dependent.^{9,10} Therefore, assuming that the trap distribution in the bulk-heterojunction has an exponential profile with characteristic temperatures, $T_{t,D}$ and $T_{t,A}$ for the donor and acceptor regions respectively. The trapped carrier densities are related approximately to the free carrier densities by⁸

$$\begin{aligned} n_t &\approx H_A \left(\frac{n_f}{N_{LUMO}} \right)^{\frac{T_{t,A}}{T}}, \\ p_t &\approx H_D \left(\frac{p_f}{P_{HOMO}} \right)^{\frac{T_{t,D}}{T}} \end{aligned} \quad (6)$$

where H_A and H_D are the densities of trap states at the acceptor LUMO and donor's LUMO respectively.

2.3 Charge Transport

The steady-state continuity and drift-diffusion equations for electrons and holes together with the Poisson equation are solved to describe the charge transport of the free carriers in the active layer, P3HT:PCBM and they are given as

$$\begin{aligned} \frac{1}{q} \nabla J_n &= PG_{tot} - (1 - P)R_n, \\ \frac{1}{q} \nabla J_p &= -PG_{tot} + (1 - P)R_p, \\ J_n &= -qn_f\mu_n \nabla V + qD_n \nabla n_f, \\ J_p &= -qp_p\mu_p \nabla V - qD_p \nabla p_f, \\ \nabla^2 V &= \frac{q}{\epsilon_0\epsilon_{r0}} (n_f + n_t - p_f - p_t), \end{aligned} \quad (7)$$

where J_n and J_p are the electron and hole current respectively, $P(T, E, x, y, z) = \int_0^\infty p(r, T, E) f(a, r) dr$ is the local probability of dissociation from polarons to free carriers, $p(r, T, E) = \frac{k_{diss}(r, T, E)}{k_{diss}(r, T, E) + k_f}$ is the probability of dissociation of the polarons into free carriers given an electron-hole separation of r in the polaron pair, $f(a, r) = \frac{4}{\sqrt{\pi}a^3} r^2 e^{-\frac{r^2}{a^2}}$ is the Gaussian distribution function describing the theoretical escape probabilities of donor-acceptor separations in a bulk heterojunction,³ V is the potential in the active region, $D_n = V_t\mu_n$ and

Table 1. List of electronic material parameters

Parameter	Symbol	Numerical Value	Remarks
Electronic bandgap	E_{gap}	1.1eV	LUMO(PCBM) = -4eV, ¹¹ HOMO(P3HT) = -5.1eV ¹²
Effective static relative permittivity	ϵ_{r0}	3.4	Based on the mixing ratio of 1:0.8, where $\epsilon_{r0}^{P3HT} = 3$ and $\epsilon_{r0}^{PCBM} = 3.9$ ¹³
Electron mobility	μ_n	$0.7 \times 10^{-4} \text{ cm}^2/\text{Vs}$	$\sim 10^{-4} \text{ cm}^2/\text{Vs}$ from experimental measurement ¹⁴
Hole mobility	μ_p	$0.7 \times 10^{-4} \text{ cm}^2/\text{Vs}$	$\sim 10^{-4} \text{ cm}^2/\text{Vs}$ from experimental measurement ¹⁴
Decay rate constant	k_f	3.2×10^4	Fitted based on the experimental short circuit current density J_{sc} and is not a free variable
Electron hole pair separation	a	1.15nm	From Koh et al ¹
Characteristic temperature of traps	$T_{t,A} (T_{t,D})$	1200K	Unique fitting parameter
Density of states of electrons (holes)	$N_{LUMO} (P_{HOMO})$	$4.2 \times 10^{22} \text{ cm}^{-3}$	Constrained fitting parameter related to $T_{t,A}$ and $T_{t,D}$
Density of states of trapped electrons (holes)	$H_A (H_D)$	$2 \times 10^{13} \text{ cm}^{-3}$	Constrained fitting parameter related to $T_{t,A}$ and $T_{t,D}$
Series Resistance	R_s	1.8Ω	Experimental measurement is $\sim 1 - 2\Omega$

$D_p = V_t \mu_p$ are the diffusion constants that are related to the thermal voltage $V_t = k_B T / q = 0.2585 \text{ V}$ at $T=300\text{K}$, and the mobilities of electrons μ_n and holes μ_p respectively.

Assuming ohmic contacts at both ends of the active layer, the boundary conditions for the carrier transport equations are then given as

$$\begin{aligned}
 n_{anode} &= N_{LUMO} \exp\left(-\frac{E_{gap}}{k_B T}\right), \\
 n_{cathode} &= N_{LUMO}, \\
 p_{anode} &= P_{HOMO}, \\
 p_{cathode} &= P_{HOMO} \exp\left(-\frac{E_{gap}}{k_B T}\right), \\
 V_{cathode} &= V_a - \frac{E_{gap}}{q}, \\
 V_{anode} &= 0,
 \end{aligned} \tag{8}$$

where V_a is the applied bias to the Ca contact of the BHJ. Solving Eqs. (1)–(7) together with the boundary conditions in Eqs. (8), the current-voltage relationship of the organic bulk heterojunction can be obtained.

3. RESULTS AND DISCUSSION

3.1 CALIBRATION WITH EXPERIMENTAL DATA

In this improved model, we are replacing the controversial reduced Langevin recombination factor by a trapping model with an exponential distribution to reflect the role of traps induced by disorder in the BHJ. Here, we utilize most of the fitted parameters (i.e. bandgap, mobilities of electrons and holes, decay rate constant and electron hole separation) by Koh *et al*¹ and adjust the values of the HOMO and LUMO density of states of the free carriers (N_{LUMO} and P_{HOMO}) and the characteristic temperature ($T_{t,A}$ and $T_{t,D}$) & density of states (H_A and H_D) of the traps. The fitted parameters are illustrated in Table 1.

Figure 1. (Color online) Comparison of the logarithmic current density $\log_{10}(J)$ [mA/cm²] versus the applied bias, V_a [V] obtained for the control cell (a) without light illumination (dark curve) and (b) with AM1.5G illumination (light curve). The solid line is the experimental curve and the circles represent the simulation results. The geometry of the POPV device is shown as an inset in (a).

We have to emphasize that even though there are now more fitting parameters, the parameters determined from fitting are fairly unique for the P3HT:PCBM system if we are to accurately match the simulation experimental data point, especially the in the maximum power region, from $V_a=0$ to V_{oc} at $V_a=0.55$ V. With the added complexity, dark current can be modeled with the concept of traps and the fit is better than the previous model which uses the controversial reduced recombination factor. Based on the fitted parameters, we plot our simulation results of the dark and illuminated J-V curve of the control structure in Fig. 1 in logarithmic scale.

From the fitting parameters, it is interesting to note that the exponential traps of P3HT:PCBM has a characteristic temperature of 1200K or ~ 100 meV. This is higher than the trap characteristic temperature of 1000K or 86meV for small molecule active layers such as CuPc:C₆₀ and SubPc:C₆₀.⁸ This is a bit unexpected for conjugated polymer such as P3HT where shallow traps tend to dominate. Therefore, we deduce that the higher than expected trap characteristic temperature is attributed to the presence of PCBM (a small molecule acceptor).

4. PLASMONIC OPV DEVICE

After calibrating our model with experimental data, we add silver nanoellipsoids in the PEDOT:PSS hole transporting layer of the control structure and perform the full optoelectronic simulation. The nanoellipsoids encapsulated in the PEDOT:PSS have a short diameter of 40nm and long axis diameter of 400nm and has a 1% coverage (i.e. 1% of the top area is covered by the nanoellipsoids) or has a volume ratio of 0.6% versus that of PEDOT:PSS. From the optical perspective, we first compare the spectral absorption in the P3HT:PCBM active layer for the control structure and the plasmonic OPV device. Figure 2(a) illustrate that the enhancement in the spectral absorption is higher for the range of solar spectrum between 2.5-3.7eV which indicates that the silver nanoellipsoids resonantly couple more light with those photon energies to the P3HT:PCBM. There is a trade-off as the absorption of the silver nanoellipsoids in PEDOT:PSS results in a slight decrease in spectral absorption in P3HT:PCBM around 2eV. To elucidate the influence of the nanoellipsoids on the polaron generation in the plasmonic OPV device, we plot the 3D contour of the polaron generation rate G and recombination rate $R_n = R_p$ as an illustration. Here, we observe that maximum polaron generation is enhanced from 1.3×10^{28} to 1.6×10^{28} due to the presence of the nanoellipsoid as shown in the circle of Figure 2(b). The non-uniform generation of polarons for the plasmonic OPV device illustrate that 3D modeling is essential to capture the localized enhancement in absorption induced by the nanoellipsoid. Besides non-uniform polaron generation, localized perturbation of carrier recombination and free /trapped carriers the concentrations due to the presence of the silver nanoellipsoid are also be captured by the 3D model.

Figure 2. (Color online) (a) Spectral absorption rate as a function of ν in [eV], and (b) Polaron Generation G , in the P3HT:PCBM layer for the plasmonic OPV device (red dashed line) and control device (black solid line). The blue dotted line ($\sim 10^{-4}$) denotes the spectral absorption in the nanoellipsoid. The circle in (b) illustrate the perturbation in G due to the presence of the nanoellipsoid.

Table 2. Control and Plasmonic OPV device electrical characteristics

Device Characteristic	Control Cell Experiment	Control Cell Simulation	Plasmonic OPV Simulation
V_{oc} (V)	0.55	0.55	0.55
J_{sc} (mA/cm^2)	9.61	9.61	9.76
Efficiency (%)	3.61	3.76	3.82
Fill Factor (%)	68	71	71

Last but not least, the addition of the optically active silver nanoellipsoid to the PEDOT:PSS layer will result in an increase in short-circuit current as reflected in the J-V curve in Fig. 3. The main electrical characteristics of the simulated plasmonic, simulated control and experimentally measured OPV device are shown in Table 2. It was observed that the short-circuit current density J_{sc} of the plasmonic OPV device increased slightly from $9.61 \text{ mA}/\text{cm}^2$ to $9.76 \text{ mA}/\text{cm}^2$ (i.e. $\sim 1.6\%$ that of the control device, while the open circuit voltage V_{oc} remains almost the same. This corresponds to a similar increase of optical absorption from $0.038 \text{ W}/\text{cm}^2$ to $0.0386 \text{ W}/\text{cm}^2$ which is $\approx 1.6\%$. As V_{oc} primarily depends on temperature, light intensity, work function of electrode and active material morphology,¹⁵ it is not expected to vary if we only add silver nanoellipsoids in the PEDOT:PSS layer. Therefore, we are confident that the 3D optoelectronic model will be able to predict the electrical characteristic of a 3D nanostructured OPV device even if the temperature, light intensity and other related parameters are changed since they are all captured in our model. We have to emphasize that our model is a substantial improvement over previous model by Koh et al¹ as the reduced Langevin recombination factor used in that model cannot account for dark current which is a major drawback as it would be impossible to fit that model to the experimental $\log_{10}(\text{J})$ -V curve as we have illustrated in this manuscript.

5. CONCLUSION

In conclusion, we have demonstrated an improved 3D optoelectronic model which can be used to predict both the optical and electrical characteristics of an OPV device incorporating 3D nanostructures for optical or device engineering purposes. As compared to the previous model with the controversial reduced Langevin recombination factor, the improved model replaces the reduced Langevin recombination factor with the description of the exponential traps. Thus, we are able to fit experimental results better as dark current due to the trap states in the exponential tail of the density of state of the carriers are considered. Using the calibrated results, we can simulate a proposed plasmonic OPV device and predict the electrical characteristics of the plasmonic based device.

Figure 3. (Color online) Comparison of the current density J [mA/cm²] versus the applied bias, V_a [V] obtained for the control cell and plasmonic OPV (POPV) device under AM1.5G illumination (light curve). The solid line is the simulation curve for the control device and the dashed lines represent the simulation result for the POPV device.

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