



On the convergence of the algorithm for simulating organic solar cells



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ABSTRACT

This paper analyzes the convergence of the numerical solution of a set of equations which contains Poisson and current continuity equations required to simulate organic solar cells under illumination and bias applied. Due to the strong nonlinearity, choosing appropriate initial guesses is a key parameter in obtaining the convergence. To establish such initial guesses, we analyzed the behavior of electrostatic potential, and electron and hole concentration profiles along the active layer as a function of generation rate of photo-induced e–h pairs, charge mobility and thickness. Based on these results, we propose simple functions to obtain the starting values for reaching the solution in an optimized number of iterations. By using this approach, the convergence can be successfully achieved for a wide range of physical parameters such as generation rate of photo-induced e–h pairs, charge mobility, and thickness. For an organic solar cell with an active layer thickness of around 120 nm, the results show that the solution at equilibrium condition, under illumination without bias applied, and under illumination with bias applied requires around 7, 9 and 5 iterations, respectively. Although the analysis was carried out using physical parameters of one of the most studied material pair: P3HT and PCBM, our proposal can be used for arbitrary organic semiconductor.

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1. Introduction

Organic solar cells have demonstrated to be attractive due to their advantages in terms of low cost and mechanical properties. So far, the bulk heterojunction (BHJ) structure, which is a randomly interpenetrating network of donor/acceptor (p- and n-type) materials in a nanoscale, has been the most efficient device architecture [1]. Performance enhancement of BHJ solar cells can be explored by simulation which is a powerful tool to enable deeper understanding of the fundamental processes and design without the need to carry out expensive technological experiments. The internal nanostructure of the active layer has been modeled by assuming that is one semiconductor with properties derived from the two materials of the blend, with electrical behavior described by the drift–diffusion equations of charge carrier current density coupled to the Poisson's equation [2–10]. When the exponential functions to describe the electron and hole concentrations are incorporated, the system to be solved take the form of a system of nonlinear second order differential equations which does not have analytical solution. In the literature, some analytical models can be found, which have been useful for describing the voltage-dependent photocurrent in BHJ polymer solar cells in very good agreements with

experiments [11–15]. However, all closed form solutions are based on at least one of the following assumptions which could restrict the accuracy under certain conditions: (a) using empirical expressions [11,12]; (b) assuming an uniform electric field across the active layer [13–15]; or (c) considering a simplified model for recombination mechanism [14,15]. To avoid making these restrictive assumptions, numerical techniques has been used to solve the system [2–10].

The numerical solution involves a discretization procedure by which the continuous equations are replaced by discrete algebraic equations and solved for three unknown functions: electrostatic potential and quasi-Fermi potentials for electrons and holes. The procedure can be carried out by steps. First, the electrostatic potential is calculated in which only the solution of Poisson's equation is necessary because the quasi-Fermi potentials for electrons and holes can be assumed equal to zero. After the convergence for the equilibrium condition is achieved, the spatial distribution of the potential calculated and the other unknown distributions initialized to zero can be used as the initial values to solve the three coupled equations at nonequilibrium with illumination turned on. In this step, the system of equations can be solved by using a coupled method which solves the discretized Poisson and continuity equations for all grid points simultaneously [7,10]. This yields the advantage of faster convergence than the decoupled method which solves the equations sequentially. However, if the initial value in the coupled method is too far from the true solution, the algorithm may fail to converge. This can occur when the device is analyzed

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under a high illumination intensity as it means a change in generation rate of photo-induced e–h pairs from zero to an specified value which can be large enough that it overshoots the solution causing the algorithm to diverge. To avoid such scenario, the convergence can be obtained by reducing the generation rate, and then it can be gradually increased until the true value is reached. Although the solution is obtained, this approach is not efficient because each step requires computer time. As an essential parameter of the numerical method, choosing appropriate initial guesses to obtain the solution is, however, rarely reported in the literature, as well as the convergence.

In order to improve the performance of the algorithm to simulate bulk heterojunction solar cells, in this work we use the coupled method and propose simple and efficient initial guesses for quasi-Fermi potentials close enough to the solution instead of using zero vectors, which have been obtained by analyzing the behavior of electron and hole concentration profiles along the thickness of the layer as a function of generation rate of photo-induced e–h pairs, charge mobility, and thickness. Finally, initial guesses for bias-applied conditions are also discussed.

2. Electrical modeling

In this section, we introduce the physical models for organic semiconductors.

2.1. Blend semiconductor

The bulk heterojunction active layer can be modeled by assuming an effective medium with its conduction and valence bands determined by the lowest unoccupied molecular orbital (LUMO) of the acceptor and the highest occupied molecular orbital (HOMO) of the donor, respectively [2]. Therefore, the effective band gap is assumed to be the energy difference between the acceptor LUMO and the donor HOMO.

2.2. Basic equations

The electrical modeling of organic solar cells is based on three coupled differential equations: Poisson's equation, and the continuity equations for the electron and hole current densities. Such equations for the steady-state can be expressed respectively as

$$\frac{\partial^2}{\partial x^2} \varphi(x) = -\frac{q}{\varepsilon} [p(x) - n(x)], \quad (1)$$

$$\frac{\partial}{\partial x} J_p(x) = -qU(x), \quad (2)$$

$$\frac{\partial}{\partial x} J_n(x) = qU(x), \quad (3)$$

where q is the elementary charge, ε is the dielectric constant of organic blend, $\varphi(x)$ is the electrostatic potential, $p(x)$ is the hole density, $n(x)$ is the electron density, $J_{n(p)}(x)$ is the electron (hole) current density and $U(x)$ is the net generation rate. In this model, only one spatial dimension is used due to the organic solar cells have a planar structure with a very small thickness (about 100 nm) compared to the lateral dimensions (typically several mm).

The above system is complemented by equations which describe the electron and hole concentrations, the electron and hole current densities, and the net generation rate.

2.3. Electron and hole concentration

By assuming Maxwell–Boltzmann statistics, electron and hole concentrations can be written respectively as

$$p(x) = n_{\text{int}} \exp\left(\frac{q [F_p(x) - \varphi(x)]}{k_B T}\right), \quad (4)$$

$$n(x) = n_{\text{int}} \exp\left(\frac{q [\varphi(x) - F_n(x)]}{k_B T}\right), \quad (5)$$

where $F_p(x)$ and $F_n(x)$ are the hole and electron quasi-Fermi potentials, respectively, k_B is Boltzmann's constant, T is the absolute temperature, and n_{int} is the intrinsic carrier density of electrons and holes, which is defined as

$$n_{\text{int}} = N_{\text{eff}} \exp\left(-\frac{E_g}{2k_B T}\right) \quad (6)$$

with the effective density of states of both the conduction and valence band, N_{eff} , and the effective band gap, E_g .

2.4. Charge transport equations

If the carrier diffusion coefficients obey the Einstein relation, the electron and hole currents incorporating both drift and diffusion of charge carriers are given by

$$J_p(x) = -qp(x) \mu_p \frac{\partial}{\partial x} \varphi(x) - \mu_p k_B T \frac{\partial}{\partial x} p(x), \quad (7)$$

$$J_n(x) = -qn(x) \mu_n \frac{\partial}{\partial x} \varphi(x) + \mu_n k_B T \frac{\partial}{\partial x} n(x), \quad (8)$$

where μ_p is the hole mobility and μ_n the electron mobility. In this model, the mobilities of hole and electron carriers are assumed to be independent of the electric field which is taken to be constant within the organic blends.

2.5. Net generation rate

In this work, we used a recombination model based on both the so-called charge transfer states [2], which is considered as a geminate recombination process [16], and bimolecular recombination explained by Langevin theory. The net generation rate of free-charge carriers can be expressed as

$$U(x) = P(x) [G + R(x)] - R(x), \quad (9)$$

where $P(x)$ is the average dissociation probability of bound e–h pairs, $R(x)$ is the recombination rate, and G is the generation rate of photo-induced e–h pairs, which is assumed to be homogeneous throughout the active layer.

Recently, it has been demonstrated that non-geminate recombination in disordered organic semiconductors can be described by free-to-trap carrier recombination [17–19]. In this study for simplicity we neglect the presence of carrier trap states and use the classical Langevin recombination approximation [2,20,21]. By using Langevin theory, the bimolecular recombination of charge carriers is given by

$$R(x) = \gamma [n(x)p(x) - n_{\text{int}}^2], \quad (10)$$

where γ is the recombination constant determined by the minimum mobility [6,22], which is defined as

$$\gamma = \frac{q}{\varepsilon} \min(\mu_n, \mu_p). \quad (11)$$

The bound e–h pair may either dissociate into free carriers or geminately decay to the ground state. The probability of e–h pair dissociation, according to Braun's model, is given by

$$p_{\text{Braun}}(x, a) = \frac{k_{\text{diss}}(x, a)}{k_{\text{diss}}(x, a) + k_f}, \quad (12)$$

where k_f and $k_{\text{diss}}(x, a)$ are the decay rate to the ground state and the dissociation rate of bound electron–hole pairs, respectively.

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