



# 2-D Modeling of Bulk Heterojunction Solar Cells With a Gaussian Shape in Donor-Acceptor Interface as Morphology

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## Abstract

In this work, we presented numerical modeling for the bulk heterojunction polymer solar cells (BHJ) based on the finite difference method to obtaining the BHJ characteristics. Our model for the BHJ, where the electron donor and acceptor materials are mixed in a solution, is two separate domains with gaussian shape interface. In this model we consider a two-dimensional geometry of thickness  $L$  on  $y$ -axis and periodic along  $x$ -axis. We assume that the rate of exciton generation to be homogenous throughout device. Some of obtained characteristics are the density of electrons and the density of the holes, current density, open circuit voltage and short circuit current density.

*Keywords:* Solar cells, Bulk heterojunction, Organic semiconductor polymer, Donor, Acceptor.

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## 1. Introduction

Organic polymer solar cell is a low cost source of renewable energy compared to traditional inorganic solar cells [1], [2]. Due to their good flexibility, they are easily mounted on a variety of substrates and have relatively acceptable durability [3]. In regular organic polymer solar cells, the donor and acceptor semiconductors are located in two separate regions with a common interface [4]. In order to improve the performance of the solar cell, the length of the active area can be increased by introduction of the bulk heterojunction (BHJ) concept as an active layer where electron donor and acceptor materials are mixed in a solution and cast into a thin film sandwiched between two electrodes [5].

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The power conversion efficiency has exceeded 9% for BHJ solar cells in recent published research. As donor polymers used in this type of structures, these polymers can be mentioned,  $C_{18}H_{28}O_2$  (MEH-PPV),  $C_{31}H_{14}S$ (P3HT). The C60 and C70 derivative PCBM is the most widely used electron-acceptor material in PSCs [6]. Anode in these types of cells is usually a metal oxide that is coated with the PEDOT: PSS layer. And the cathode is made of a metal with a low work function, such as aluminum [7].

## 2. Active layer structures and governing equations

The photon absorption in the solar cells yields an exciton (bound electron-hole pair) that is transmitted to the donor-acceptor interface by diffusion processes. The dissociation of the electron-hole pair due to electric field, produces free charge carriers and these free carriers have to be transported through their respective phases to the electrodes (drift processes) in order to be extracted. The decay of exciton is one of the possible mechanisms of loss, and the second mechanism is the recombination of free charge carriers. For organic bulk hetero junctions, in 2D drift-diffusion simulation the mediums are separated [8]. This approach permits the influence of morphology with gaussian shape for boundary of effective medium. Although multidimensional drift-diffusion simulations are possible, this work will only discuss the 2D version. The two-dimensional equations describing the electric field and its dependent potential and the charge carrier densities are the Poisson equation and continuity equations that consider the processes of generation, diffusion and recombination that can be solved by applying boundary conditions. The Poisson equation for electric potential  $\phi$  is [9]:

$$\nabla^2 \phi(x, y) = -\frac{e}{\epsilon \epsilon_0} (p(x, y) - n(x, y)) \quad (2.1)$$

Where  $e$ ,  $\epsilon$  and  $\epsilon_0$  are electron charge, dielectric constant and permittivity of vacuum,  $n$ ,  $p$  stand respectively for the concentrations of electrons and holes and  $e = 1.6 \times 10^{-19}$  C. As we interest the study of current density with applied voltage (J-V curves), we focus on steady-state equations. The current continuity equations for electron and hole:

$$\nabla \cdot J_n(x, y) = -e(G - R) \quad (2.2)$$

$$\nabla \cdot J_p(x, y) = +e(G - R) \quad (2.3)$$

$G$  is the generation rate of excitons and  $R$  is the recombination rate for the free carriers and  $G-R$  is the net generation rate of free carriers and  $J_{n(p)}$  is the electron(hole) current density. The current densities in terms of both diffusion and drift processes are:

$$J_n = -en\mu_n \nabla \phi + eD_n \nabla n \quad (2.4)$$

$$J_p = -en\mu_p \nabla \phi - eD_p \nabla p \quad (2.5)$$

$D_{n(p)}$  and  $\mu_{n(p)}$  are respectively the diffusion constant and mobility of electrons(holes) in the acceptor and donor domains, which are assumed to obey the Einstein relation.

$$\frac{D_n}{\mu_n} = \frac{D_p}{\mu_p} = \frac{k_B T}{e} \quad (2.6)$$

where  $k_B$  is Boltzmann's constant and  $T$  is the absolute temperature.

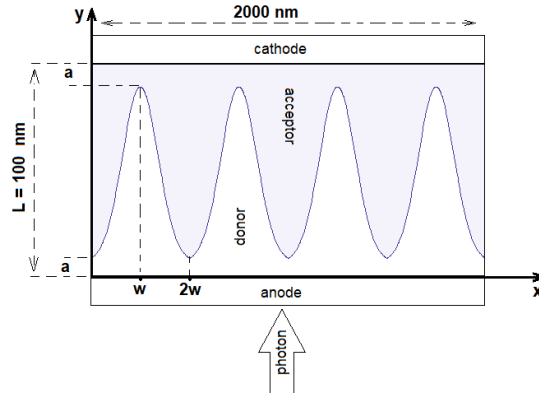


Figure 1: Donor-Acceptor interface.

### 3. The boundary conditions and results

Excitons are created in the donor domain, and they diffuse towards a donor-acceptor interface, where allows the splitting into free charges. Fig.1 shows a gaussian shape for interface of donor and acceptor domains that we considered in our simulation as morphology.

$$y = \frac{a(2.72 + 1) - L}{(2.72 - 1)} + \frac{2.72(L - 2a)}{(1 - 2.72)} \text{Exp} \left( -\frac{(x_i - w)^2}{w} \right)$$

$$(2i)w \leq x_i \leq (2i + 2)w \quad , \quad i = 0, 1, 2, 3, \dots \quad (3.1)$$

Where 2.72 is the base of the natural logarithm,  $a=20$  nm and  $w$  is half-width of donor and acceptor domain is close to the mean exciton diffusion length fixed to 8.5 nm and  $L=100$  nm is thickness of layer.

According to the Metal-Insulator-Metal model, we consider the potential between electrodes to be equal to the difference between an effective bandgap  $E_{gap}$  (between the HOMO level of the donor and the LUMO level of the acceptor) and an applied voltage  $V_{ap}$ . And we also assume there is not barrier at the electrodes.

$$\phi(y = L) - \phi(y = 0) = \frac{E_{gap}}{e} - V_{ap} \quad (3.2)$$

$L=100$  nm is Thickness of medium. Using Boltzmann statistics, the boundary conditions at cathode are:

$$p(y = L) = N_v \text{exp} \left( -\frac{E_{gap}}{k_B T} \right)$$

$$n(y = L) = N_c \quad (3.3)$$

And at anode:

$$n(y = 0) = N_c \text{exp} \left( -\frac{E_{gap}}{k_B T} \right)$$

$$p(y = 0) = N_v \quad (3.4)$$

Where  $N_{c(v)}$  is the effective density of states of the conduction(valence) band and  $k_B=1.38 \times 10^{-23}$  Kg $m^2/s^2$ K and  $T=300$  K. Due to the fact that the extraction or generation of carriers in cathode and anode metal electrodes is not completely efficient, a limited level should be considered for the rate of recombination and extraction of carriers. We have for recombination rate [10]:

$$R = \frac{e(\mu_n - \mu_p)}{\epsilon \epsilon_0} \cdot \frac{k_d}{k_d + k_f} \times n \times p \quad (3.5)$$

$k_d$  is rate of electron-hole pair dissociation in transfer exciton and  $k_f$  is a constant that shows the decay rate of the bound electron-hole pair to the ground state.

$$k_d = \frac{3\gamma}{4\pi r^3} \cdot \frac{J_1(2\sqrt{-2b})}{\sqrt{-2b}} \cdot \exp\left(-\frac{U_{Col}}{k_B T}\right)$$

$$\gamma = \frac{e(\mu_n + \mu_p)}{\epsilon\epsilon_0} \quad (3.6)$$

$J_1$  is the Bessel function of order 1,  $r$  is average distance of electron-hole pair in exciton and  $U_{Col} = \frac{e^2}{4\pi\epsilon\epsilon_0 r}$  is the electron-hole pair binding energy. For  $b$  we have

$$b = \frac{e^3}{8\pi\epsilon\epsilon_0 k_B^2 T^2} \cdot \frac{\phi(L) - \phi(0)}{L}$$

In order to reduce the number of unknown parameters in the model, we fix some of them to the values commonly found in the literature, and listed in Table 1. For simplicity we assume that the generation rate  $G$  is constant. However in some cases  $G$  is derived by solving the diffusion equation for excitons.

From equations (2.2), (2.3) and (2.4), (2.5), equations (3.7), (3.8) are obtained.

$$\nabla \cdot (-en\mu_n \nabla \phi + eD_n \nabla n) = -e(G - R) \quad (3.7)$$

$$\nabla \cdot (-en\mu_p \nabla \phi - eD_p \nabla p) = +e(G - R) \quad (3.8)$$

According to the boundary conditions the equations of (2.1), (3.7) and (3.8) are solved by the finite difference method and  $n$ ,  $p$ ,  $\phi$  are obtained. Then, the current densities are obtained from them. Spatial average of  $y$ -component of the currents yields total current  $J = \langle J_{py} \rangle + \langle J_{ny} \rangle$  and is shown in fig.2.

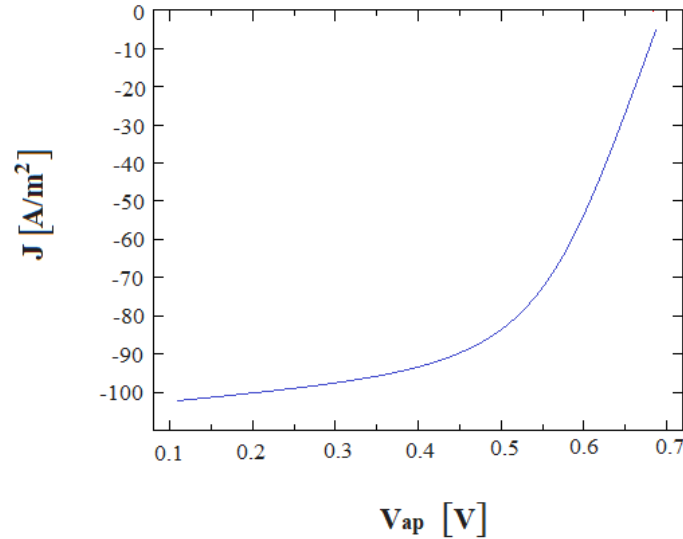


Figure 2: calculated total current density.

Figure 2 shows the average behavior of the total current density, which is in agreement with [11]. And fig.3 shows electron(hole) density as function position along the thickness of the medium. Figure 3 indicates that the electron(hole) density increases(decreases) from the anode to the cathode, which is in agreement with [12]. Table 1 [12] shows the values used in this work.

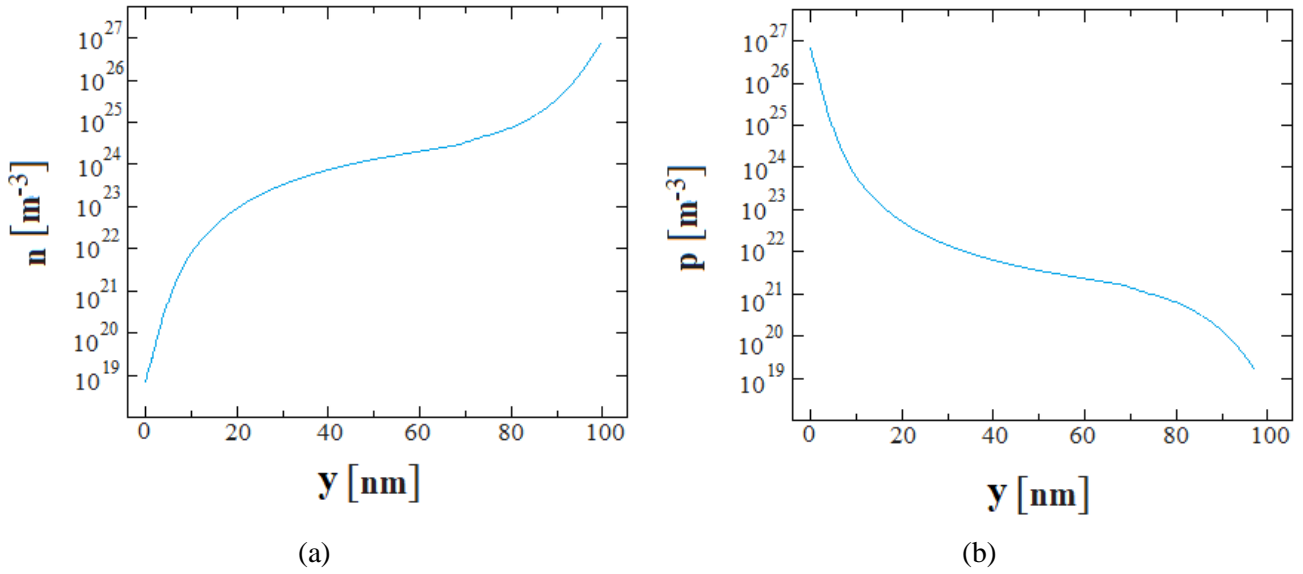


Figure 3: Electron(hole) densities as function of y component of position.

Table 1: The value of the parameters

Parameter	Value	Unit
$\mu_n$	$2 \times 10^{-8}$	m <sup>2</sup> /Vs
$\mu_p$	$2 \times 10^{-8}$	m <sup>2</sup> /Vs
$r$	1.8	nm
$\epsilon$	3.5	-
$E_{\text{gap}}$	1.0	eV
$G$	$7.4 \times 10^{27}$	m <sup>-3</sup> s <sup>-1</sup>
$N_c$	$4 \times 10^{25}$	m <sup>-3</sup>
$N_v$	$4 \times 10^{25}$	m <sup>-3</sup>
$k_f$	$2 \times 10^4$	s <sup>-1</sup>

#### 4. Conclusion

It should be noted that the values of parameters for solar cells are entirely dependent on the solar cell fabrication. So that values calculated in different numerical tasks are not necessarily equal to each other. However, the behavior of the obtained graphs must be consistent with the practical data and numerical data of other works. Figure 2 shows the average behavior of the total current density, which is in agreement with literature. Figure 3 indicates that the electron(hole) density increases(decreases) from the anode to the cathode as expected. These calculations show that the proposed model can describes BHJ solar cell behavior. For light intensity about 1000 W/m<sup>2</sup>, the open circuit voltage  $V_{OC}=0.6$  V, short circuit current  $J_{SC}=30$  A/m<sup>2</sup>, fill factor  $FF \approx 4\%$  and power

conversion efficiency  $\eta \approx 7\%$  are calculated.

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