

The influence of nanostructure on polymer-based optoelectronic device functioning: A computer simulation study

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ABSTRACT

During the last years it has been clear that it is important to understand and control the nanostructure of the active polymer layer used in optoelectronic devices, like polymer diodes, solar cells or field effect transistors. Several experimental studies have shown that the nanostructure of polymer thin films used in these optoelectronic devices depends on the conditions used to deposit the polymer layer between the electrodes. As a result, in solid state conjugated polymer chains tend to be stacked and aligned relative to the electrodes creating domains with different sizes that influence the performance of these devices. To understand how the spatial arrangement of polymer chains affects the functioning of optoelectronic devices, we performed computer simulations using our mesoscopic model based on a generalized dynamic Monte Carlo method. We focus our study on the influence of the nanomorphology on the electric properties of polymer light emitting diodes. Our results show that for a pristine polymer layer and in the presence of ohmic contacts between the electrodes and the polymer layer, the electric properties of the device, namely current density, charge density, internal electric field and the number of charges that undergo recombination strongly depend on the polymer morphology at nanoscale.

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1. Introduction

Although electronic devices with an active layer made of an organic semiconductor have reached the commercial market, namely in the display industry, the application of this type of materials to other devices, like field effect transistors or solar cells is still in a premature stage. In the case of these devices the morphology of the organic semiconductor seems to play a major role in their performance, especially when the semiconductor is made of a conjugated polymer [1,2].

There are several experimental results that suggest that the electronic and optoelectronic behaviours of polymer-based devices are influenced by the morphology of the polymer at nanoscale. Measurements of the electroluminescence across a PPV-derivative film by the scanning tunneling microscope showed a non-uniform emission which was attributed to changes on the spatial arrangements of polymer chains at nanoscale [3]. This assumption is supported by other studies that showed that in spin-coated films, and depending on the experimental conditions used to deposit the film, most of the polymer chains tend to be aligned parallel to the electrode's

surface in those films and there are domains where polymer chains have perpendicular or random orientations [4,5]. These different nanomorphologies of the polymer film affect not only the optical properties, namely the polarization and intensity of light emission from these films [5,6], but also the electrical ones, like charge mobility [7–9], which strongly affects the overall functioning of polymer-based devices.

In solid state, the conjugation of long polymer chains is disrupted by the presence of kinks, twists or defects that lead to the chain packing [10]. At the end, each polymer film can be seen as an assembly of conjugated strands with different conjugation lengths [11] forming domains with a specific orientation of the strands relative to the electrode's surface.

Most of the theoretical studies performed to understand the functioning of polymer-based devices at nanoscale are based on the work developed by Bäessler [10] who considers charge injection and transport as a result of charge hopping processes to or between localized states [12]. However, it was showed recently at experimental [13] and theoretical [14] level that charge mobility along conjugated segments can contribute to charge transport throughout the polymer network. Since in a real polymer film there are a large number of domains with conjugated segments with different orientations, it is difficult to obtain from the experiments the influence of each domain on the function of polymer-based devices. It is in this context that computational experiments can have an added value, since they allow us to study the influence of each individual domain on the device functioning. For that purpose we

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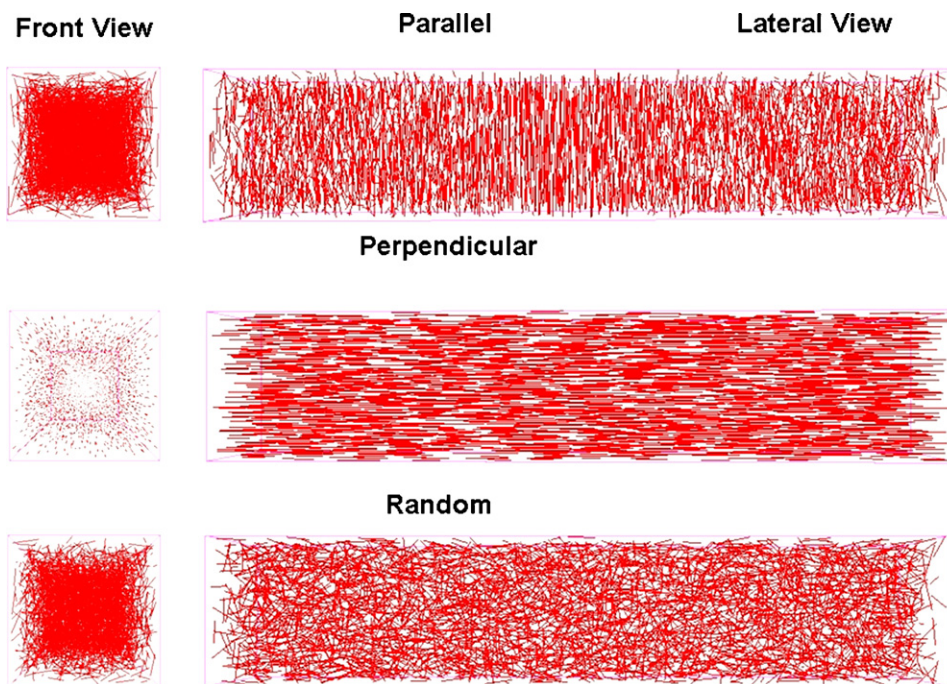


Fig. 1. Representation of the polymer networks with parallel, perpendicular and random morphologies viewed in the direction perpendicular (front view) and parallel to the electrode's surface. The lines represent the molecular axis of the conjugated segments.

use our mesoscopic model, based on a generalized dynamic Monte Carlo method, to study the influence of the nanomorphology on the functioning of polymer light emitting diodes (PLEDs) with poly(p-phenylene vinylene) (PPV) as the active component. Our model includes explicitly the arrangement of PPV strands at nanoscale as well as the intramolecular charge transport and the molecular properties of the polymer obtained by atomistic calculations.

2. Computational model and simulation conditions

In order to understand how the different conjugated segment arrangements relative to the electrode's surface influence the functioning of a PLED, we started to mimic these polymer morphologies by creating 3D-networks with PPV conjugated segments parallel, perpendicular and randomly oriented relative to the electrode's surface. Each polymer network is built by placing randomly in the gap between two planar electrodes, separated 100 nm from each other (model axis), straight conjugated segments whose length is taken from a gaussian distribution of segment lengths considering a mean value of 7 monomers [11,15]. In our model we assume that each conjugated segment can be seen as a rigid rod, where the minimum distance allowed between two polymer segments and between those and the electrodes is 0.650 nm, as obtained from atomistic calculations [11,15]. Fig. 1 shows the three polymer morphologies considered in our simulations, where each line represents the molecular axis of the polymer segments with the parallel, perpendicular and random orientations relative to the electrode's surface.

Our mesoscopic model includes the processes of charge injection, transport, recombination and collection by the electrode opposite to the injection one, that are on the base of a PLED functioning and takes into account the atomistic results obtained by Ramos and co-workers [11,15]. These results showed the formation of a polaron-type defect after a charge be injected in a conjugated segment due to electron-lattice coupling. When the strength of the local electric field (i.e. the sum of the applied electric field, the electric field created due to space charge distri-

bution and the electrode polarization) along the segment axis is smaller than the threshold for intramolecular polaron mobility, the injected charge moves towards the segment central region otherwise it moves to the segment end favoured by that electric field (i.e. intramolecular charge transport). From that position, the created negative/positive polaron can then hop to another segment (i.e. intermolecular charge transport), depending on the difference between the electron affinity (EA)/ionization potential (IP) of the conjugated polymer segments involved obtained from atomistic calculations [11,15], as well as the strength of the electric field.

In our mesoscopic model the hopping rates associated to the electronic processes of charge injection/collection from/by the electrodes and intermolecular charge hopping within the 3D-polymer network are given by:

$$w_{ij,\text{hop}} = w_{0,\text{hop}} \times f(r_{i,j}) \times g(\Delta E_{i,j}) \times h(\theta) \quad (1)$$

where the term $w_{0,\text{hop}}$ represents the *attempt-to-escape* frequency while the following terms represent the influences of the hopping distance ($f(r_{i,j})$), the energy barrier height that a charge has to overcome between hopping sites ($g(\Delta E_{i,j})$) and the angle between the local electric field direction and the hopping direction ($h(\theta)$).

In our simulations we consider that the electrode/polymer interfaces are perfectly ohmic so that the main factor affecting bipolar charge injection and transport is the arrangement of the polymer segments within the network. When two charges of opposite sign meet in the same polymer segment, they can recombine if the local electric field along the segment axis is not strong enough to keep the two charges apart.

The time evolution of all electronic processes is obtained using the first reaction method. For each electronic process associated with a charge (e.g. injection/collection from/by the electrode, hopping between neighbouring segments, recombination) a time of occurrence is attributed, and the electronic process that takes place at each Monte Carlo step is the one that presents the smallest time of occurrence. During the simulation we follow charge percolation throughout the polymer network as a function of time until the steady state is reached.

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