

Modelling the effects of molecular arrangements in polymer light-emitting diodes

Marta M. D. Ramos* and Helena M. G. Correia

Departamento de Física, Universidade do Minho, Campus de Gualtar, 4700-057
Braga, Portugal

E-mail: *marta@fisica.uminho.pt

Abstract. In order to understand how to enhance the performance of polymer light-emitting diodes (PLEDs), we used a mesoscopic hopping model, taking into account molecular properties and polymer morphology, to investigate the impact of a number of conjugated polymers and molecular arrangements on the functioning of single layer devices. The model is applied to devices with the active polymer consisting of poly(p-phenylene vinylene) (PPV) and PPV derivatives with stiff conjugated segments having their long axis oriented parallel and perpendicular to the electrode surfaces as well as randomly oriented, which are three of the molecular arrangements that can be obtained experimentally at microscopic scale in solution-processed conjugated polymer thin films.

The model provides insight into current efficiency, charge distribution, internal electric field and consequently recombination throughout the polymer layer. We found that the details of molecular arrangement crucially affect the distribution of recombination events far from the electrodes and its field-dependence, which has implications for the efficiency of PLEDs. In particular, we found a variation of recombination efficiency in the bulk of uniform ordered polymer films depending on the molecular alignment relative to the electrode surfaces. It turns out that molecular orientation perpendicular to the electrodes increases recombination in the centre of the polymer film as compared to the case of parallel orientation. We conclude that the orientational alignment perpendicular to the electrode surfaces might be a viable strategy towards efficient polymer-based LEDs.

PACS numbers: 73.63.-b, 73.61.Ph, 78.20.Bh, 78.66.Qn

1. Introduction

Since the first report of electroluminescence in poly(p-phenylene vinylene) (PPV) in 1990 [1], much research has focused on PPV and its derivatives in the context of polymer light-emitting diodes (PLEDs). Although the optimization of PLEDs has been made without recourse to evaluating the molecular arrangements of the conjugated polymer films, it has become clear that details of the morphology of the molecules have a large impact on charge carrier mobilities [2], which ultimately should affect device efficiency.

Self-organization in solution-processed conjugated polymer thin films results in complex microstructures, in which highly ordered domains are embedded in the disordered matrix [3]. Depending on the processing conditions, the stiff-chain conjugated segments within the ordered domains can adopt two different orientations (parallel and normal to the substrate [4, 5]) which should affect device performance. Therefore, it is crucial to understand the effect that molecular arrangement has on the performance of these polymer based devices, to achieve morphological control of individual polymer chains so that the ensemble of polymer molecules can be organized to yield the desired device performance. Since it is difficult in the experiments to isolate the effects of each film region with different molecular arrangements, modelling is required to understand how different molecular alignments relative to the planar electrodes influence recombination efficiency and recombination distribution in PLEDs. Despite the extensive literature published on macroscopic and microscopic modelling of organic electroluminescent devices, recently reviewed by Walker et al. [6], very little work has been carried out using microscopic models in which the polymer film morphology is explicitly included [7, 8, 9, 10, 11, 12, 13] and the majority of them [7, 8, 9, 10] does not include parameters related to material chemistry.

In a previous paper [13] we used a mesoscopic hopping transport model, in which the polymer film morphology and the intra-molecular properties of the polymer molecules are explicitly included, to assess the influence of cyano-substitution on the properties of single layer spin-coated PPV light-emitting diodes. The aim of the present work is to extend the application of this model to other morphologies of PPV-based polymers obtained by different experimental techniques. In particular we discuss the effects of molecular arrangements parallel, perpendicular and randomly oriented relative to the electrode surfaces on current flow, charge accumulation and recombination within the polymer. The additional effect on internal electric field and recombination profiles is also considered.

2. Modelling and simulation details

In thin films of conjugated polymers commonly used in PLEDs, each polymer macromolecule consists of a large number of stiff-chain segments with a conjugation length typically less than 10 monomer units [5, 11, 14]. As a result, each conjugated segment within the polymer macromolecule, linked to other conjugated segments by

twists or kinks, behaves like a separate straight chain. Therefore, these polymer films sandwiched between two planar electrodes can be modelled as a three-dimensional network of straight conjugated chains with variable chain length. The straight chains will be distributed within the gap between the electrodes according to the desired morphology.

In this work three different film morphologies are considered. In one of them all chains have their long axis parallel to the electrode surfaces but a random orientation to each other. In another the straight chains are aligned perpendicular to the electrode surfaces and finally we examined the case in which each chain in the network points in a different direction (orientational disorder). In all these morphologies the chain backbone planes have a random orientation and the inter-chain distance between any two chains varies randomly from a minimum value, which corresponds to the co-planar configuration. The random inter-chain distances and the random angles are both taken from a uniform distribution.

The building of the polymer networks described above requires information from the experiments concerning the length per monomer unit, the minimum inter-chain distance for co-planar configuration and the distribution of conjugated segment lengths, that are not generally well known. We therefore approach this problem with data coming from atomic scale calculations using the CHEMOS code [15, 16] and assuming a Gaussian distribution of straight chain lengths with a mean value of 5.

Given these realizations of the polymer structure, we can carry out computer experiments in which electrons and holes are injected into the polymer layer from opposite electrodes. The distribution of conjugated chains within the polymer film results in a distribution of electronic states and the inter-molecular bipolar charge transport can then be modelled by the hopping among electronic states of neighbouring chains. Because of Coulomb blockade, we assume that there is no more than one electron or hole on each chain. Therefore, holes are transported in the highest occupied molecular orbitals, whereas electrons are transported in the lowest unoccupied molecular orbitals.

In order to simulate the bipolar charge transport in PLEDs based on PPV with and without chemical substitution by electron donor groups (methoxy substitution) and electron accepting groups (cyano substitution), whose chemical structures are shown in figure 1, it is necessary to investigate their individual molecules to get estimates of the ionization potential and the electron affinity as a function of the chain length. It is also necessary to determine the most energetically favourable position of the injected charge over the chain and its dependence on the strength of the electric field along the chain. In previous work already published [11, 17, 18, 19] we show that in PPV, cyano-PPV and dimethoxy-PPV the charging of a chain results in a charge-induced defect in the chain backbone (charge dressed with lattice distortion), which is localized at the centre of the chain if the electric field applied along it is lower than the field needed for intra-molecular charge mobility, otherwise the injected charge moves toward the chain-end favoured by the electric field. The results of such atomic scale calculations concerning the ionization potential and electron affinity of chains with different number of monomer units and the

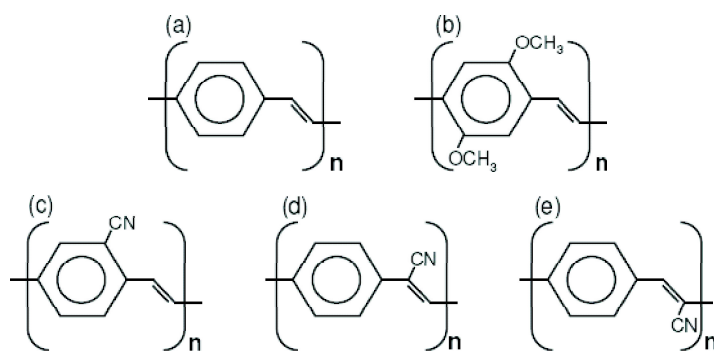


Figure 1. The chemical structures of the investigated materials: (a) poly(p-phenylene vinylene) (PPV); (b) poly(2,5-dimethoxy-para-phenylene vinylene) (DMeOPP); (c) poly(2-cyano-para-phenylenevinylene) (2-CN-PPV); (d) poly(7-cyano-para-phenylenevinylene) (7-CN-PPV); (e) poly(8-cyano-para-phenylenevinylene) (8-CN-PPV).

electric field threshold for electron and hole mobility along the chains are summarized in figure 2 and Table 1. These results will be incorporated in our mesoscopic approach

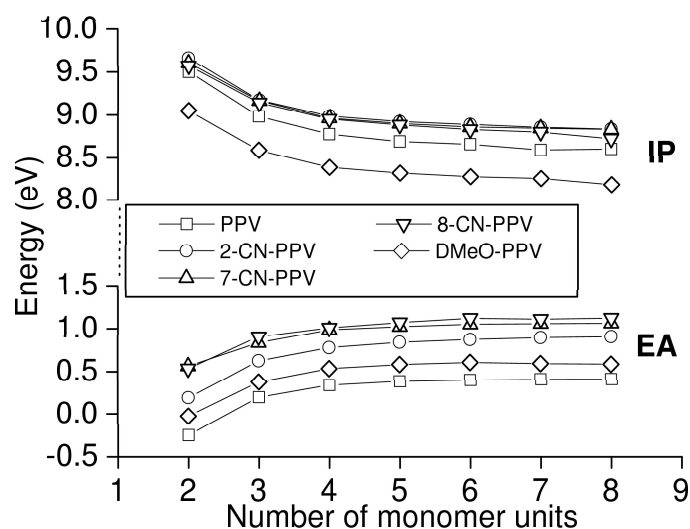


Figure 2. Ionization potential (IP) and electron affinity (EA) as a function of the number of monomer units in the chain for PPV, 2-CN-PPV, 7-CN-PPV, 8-CN-PPV and DMeO-PPV [11, 18, 19].

of bipolar charge transport in PLEDs as input data.

The sequence of charge processes leading to light emission in PLEDs is the injection of bipolar charge carriers into the polymer chains bound to the electrodes chosen randomly, their hopping-type transport through the polymer network and

Polymer	Electric field (MV/cm)	
	Q = +1	Q = -1
PPV	2	1.55
2-CN-PPV	2.067	2.69
7-CN-PPV	2.249	2.41
8-CN-PPV	2.218	2.393
DMeO-PPV	5.628	3.435

Table 1. Electric field threshold for the mobility of the injected charge (electron and hole) along the chains of the investigated materials.

recombination. A perfect ohmic contact between the electrodes and the chains bound to them is assumed in the present model.

Since the balanced charge injection from both electrodes is crucial for high device efficiencies, a constant injection rate of one electron-hole pair per computer time-step is assumed in this work. It is not difficult to generalize this approach to include the dependence on applied electric field and the effects of energetic disorder at electrode/polymer interface, but this is not done in the present paper.

Under the influence of the local electric field, the injected charges move along the chains to the position that is energetically more favourable before they can jump to a neighbouring chain. The jump rate between two chains i and j , W_{ij} , is assumed to be [8]:

$$W_{ij} = W_0(\cos \theta + 1) \exp\left(-\frac{R_{ij} - R_0}{R_0}\right) \times f(\Delta E_{ij}) \quad (1)$$

where

$$f(\Delta E_{ij}) = \begin{cases} \exp[-\Delta E_{ij}/(k_B T)], & \text{for } \Delta E_{ij} > 0 \\ 1, & \text{for } \Delta E_{ij} < 0. \end{cases}$$

where the attempt-to-jump frequency, W_0 , is a material constant, θ is the angle between the electric force vector on the charge and the position vector along the jumping path, R_{ij} is the jumping distance, R_0 is the minimum inter-chain distance allowed, k_B is the Boltzmann factor, T is the temperature and ΔE_{ij} is the energetic barrier that the charge carrier has to overcome during the jump. The value of ΔE_{ij} depends on the difference between electron affinities (for hole transport) or ionization potentials (for electron transport) of the chains involved in the jumping process as well as on the effect of the local electric field on such activation energy. The trajectories of the charges within the polymer network arise from the constraint that the probability for charge carriers to jump between two neighbouring chains, defined by

$$P_{ij} = \frac{W_{ij}}{\sum_{i \neq j} W_{ij}} \quad (2)$$

is greater than 90% and the jump rate is greater than 10^{-5} .

Recombination occurs during the simulations whenever two oppositely charged carriers meet on the same chain. No inter-chain recombination was considered in this work.

In the present work, all the polymer networks built have a thickness of 100 nm and 11300 straight chains in a polymer cell with the volume of 40000 nm³. Periodic boundary conditions are applied along the directions parallel to the electrode surface for the construction of the entire polymer film. When we change the polymer material in the network, we do so at constant number of chains. As a consequence, there is a small density change that should not have significant effect on the interpretation of the following results.

3. Results and discussion

When multiple electron-hole pairs are injected in the polymer network at constant rate, some of the injected charges cross the polymer layer to carry a current, others are in transit inside the polymer and contribute to the space charge, whereas others recombine and only those which recombine radiatively far from the electrodes are able to contribute to the light output. Therefore, the competition between current flow, charge accumulation and recombination should affect the overall device efficiency.

Our results concentrate here on two factors: the effects of molecular properties and the effects of molecular alignment relative to the electrode surfaces.

We address first the effect of the external applied electric field on conduction across the polymer network (which is measured by the fraction of the injected charge reaching the collecting electrode) because our results can be easily compared with experimental data obtained for single-layer PPV light-emitting diodes [20]. The steady state results are shown in figure 3. These results show several general features, irrespective of the polymer chemistry. First, the current efficiency increases as the strength of applied electric field increases for all the polymer morphologies considered, because the electric field strongly enhances the mobility of both holes and electrons. This result is in agreement with the experimental observations in MEH-PPV [21]. Second, the current efficiency is similar for electrons and holes, which suggests that both charge carriers have comparable mobilities in PPV-based polymers in agreement with the conclusion drawn by Scott et al. [22] from experiments in MEH-PPV diodes. Third, the current efficiency for the molecular alignment parallel to the electrode surface exhibits the typical non-linear behaviour of current-voltage characteristics of spin-coated PPV diodes [20], whereas no significant deviations from linearity was predicted for molecular alignments perpendicular to the electrode surfaces and randomly oriented. Besides, when the molecular alignment is parallel to the electrode surfaces, the current efficiency appears to saturate for higher applied electric field. As the field becomes stronger the activation energy for inter-chain hopping is reduced, leading to the case of no energetic disorder at all for which the saturation seems to occur.

The chemical substitution of PPV by methoxy groups leads to a decrease in current

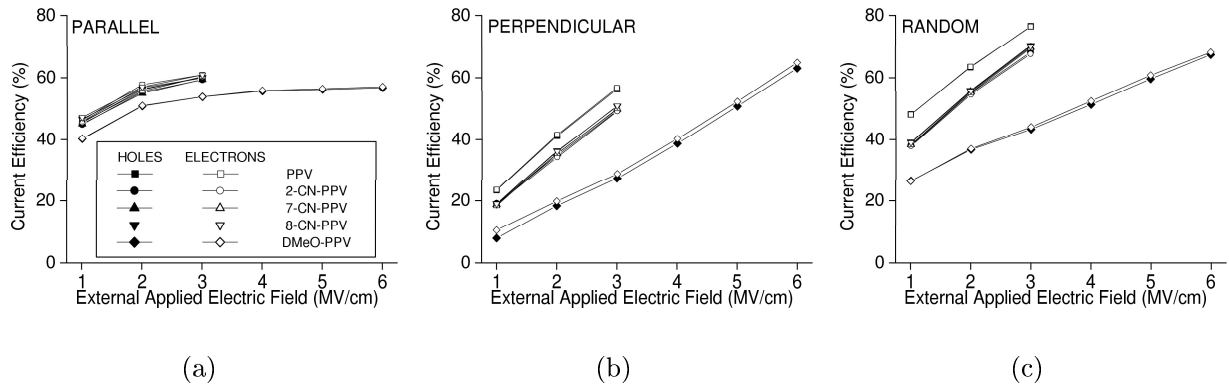


Figure 3. Current efficiency for electrons (open marks) and holes (closed marks) through PPV, CN-PPV (with the cyano substitution in positions 2, 7 and 8) and DMeO-PPV as a function of the external applied electric field, for the following chain alignments relative to the electrode surfaces: (a) parallel, (b) perpendicular and (c) random orientation.

efficiency relative to PPV regardless of the polymer morphology considered. The cyano substitution of PPV only affects current efficiency in polymer morphologies which do not have a molecular alignment parallel to the electrode surfaces, the effect being more pronounced for the random orientation.

From calculations for single-carrier diodes, with the same polymer as active material, we conclude that the mobility of both holes and electrons increases as their concentration increases. This result is in agreement with experiments [23] and numerical results obtained by Pasveer et al. [24].

The accumulation of electrons and holes in transit inside the polymer network at the steady state is shown in figure 4.

The most important feature that we find is that less than 7% of the injected charge is accumulated within the PPV-based polymers and the amount of accumulated charge does not vary significantly neither with the strength of applied electric field, nor with the polymer chemistry, but depends on the morphology of the materials. These results are in agreement with the experimental findings of essentially trap-free charge transport for PPV derivative samples [22]. The different accumulation of electrons and holes in DMeO-PPV for the polymer morphology that has chain arrangements perpendicular to the electrode surfaces is mostly dictated by the large difference between the electric field threshold for their mobility along the chain.

The effect of polymer morphology on the distribution of electrons and holes inside the polymer network in the steady state is illustrated in figure 5 for 8-CN-PPV. Similar charge distributions are obtained for PPV and DMeO-PPV.

As may be expected for essentially trap-free materials, most carriers accumulate in the region close to the collecting electrode. The space charge effects in PPV and its derivatives are quite visible on the dramatical changes in the internal electric field

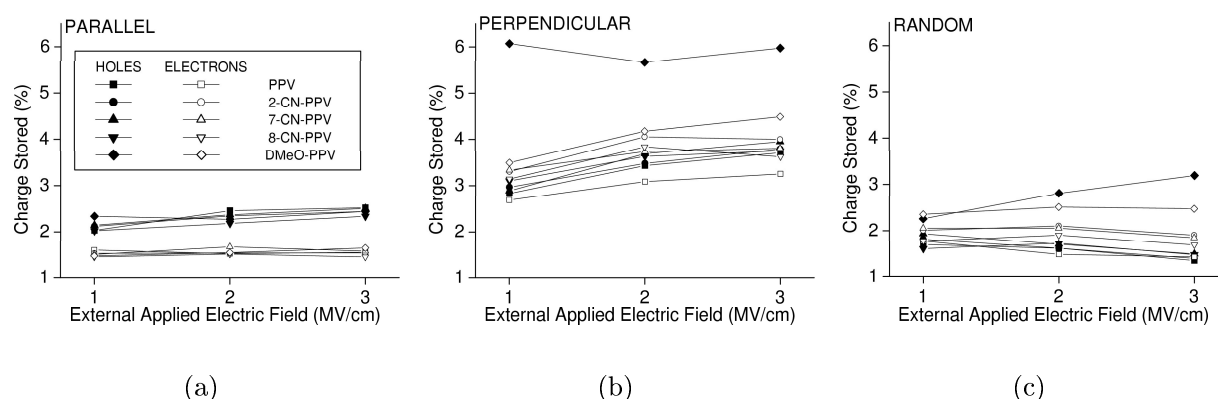


Figure 4. The proportion of injected charge (electrons and holes) that is accumulated within the PPV, CN-PPV (with the cyano substitution in positions 2, 7 and 8) and DMeO-PPV networks as a function of the external applied electric field, for the following chain alignments relative to the electrode surfaces: (a) parallel, (b) perpendicular and (c) random orientation.

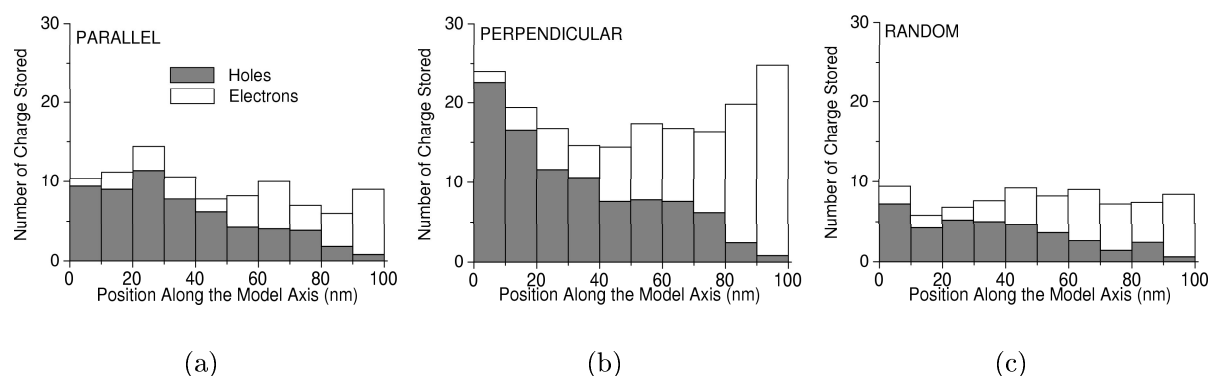


Figure 5. Electron and hole distribution inside 8-CN-PPV network in the steady state for an external applied electric field of 3 MV/m and the following chain alignments relative to the electrode surfaces: (a) parallel, (b) perpendicular and (c) random orientation.

along the model axis perpendicular to the electrode surfaces (see figure 6). There is an increase of the internal electric field in the regions close to the electrodes where the internal electric field becomes larger than the applied field, whereas the field in the bulk reaches values lower than the applied field and the field gradient in that region is quite smaller.

This is an important result because it shows how much the internal electric field is affected by the interplay between the amount of electrons and holes accumulated within the polymer and their distribution inside the network. The internal electric field profile at the steady state seems to be weakly dependent on the polymer chemistry, but it is more sensitive to change in polymer morphology.

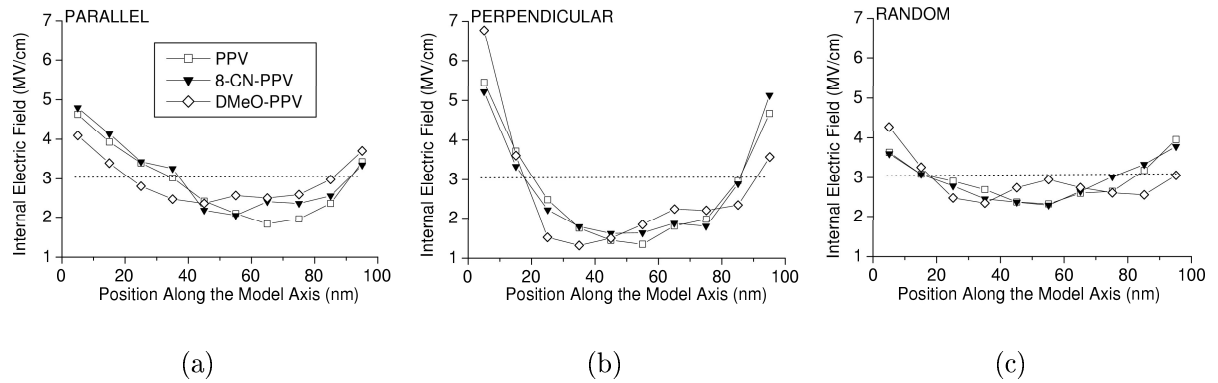


Figure 6. The internal applied electric field distribution along the model axis perpendicular to the electrode surfaces for PPV (squares), 8-CN-PPV (inverted triangles) and DMeO-PPV (diamonds) and the following chain alignments relative to the electrode surfaces: (a) parallel, (b) perpendicular and (c) random orientation. These results were obtained using an external applied field of 3 MV/cm which is represented by the dotted line.

The evolution in time of the internal electric field alters the percolation of the injected charge through the polymer network, which ultimately affects the spatial distribution of the recombination events. Therefore, similar electric field profiles predicted for PPV based polymers at steady state does not mean that their recombination profiles will also be similar.

Although the energetic disorder in PPV and CN-PPV is similar and the electric field needed for electron and hole mobility along the chains is slightly different, no significant difference was predicted for their recombination distribution profile for any of the molecular arrangements considered in this work. Figure 7 shows the effect of the external applied electric field on recombination distribution for 8-CN-PPV. The behaviour of PPV was found to be quantitatively different but qualitatively identical, indicating that small differences in the electric field threshold for intra-molecular mobility of electrons and holes has very little effect on the recombination profile for the same external applied electric field.

For PPV and CN-PPV, the recombinations that occur within the bulk of the polymer far from the electrodes, which are mainly responsible for PLED efficiency, vary only slightly with the applied field in the cases of perfect alignment either parallel or perpendicular relative to the electrode surfaces and reach saturation at large values of the applied field for the molecular alignment parallel to the electrodes. This latter result may explain the maintenance of high luminous efficiency at high applied field for single layer PLED based on spin-coated PPV [20]. The orientational disorder does not affect significantly the recombination distribution in the central region of the film, but only results in the reduction of recombination intensity as the applied field increases.

Figure 8 shows calculated recombination distribution profiles inside DMeO-PPV

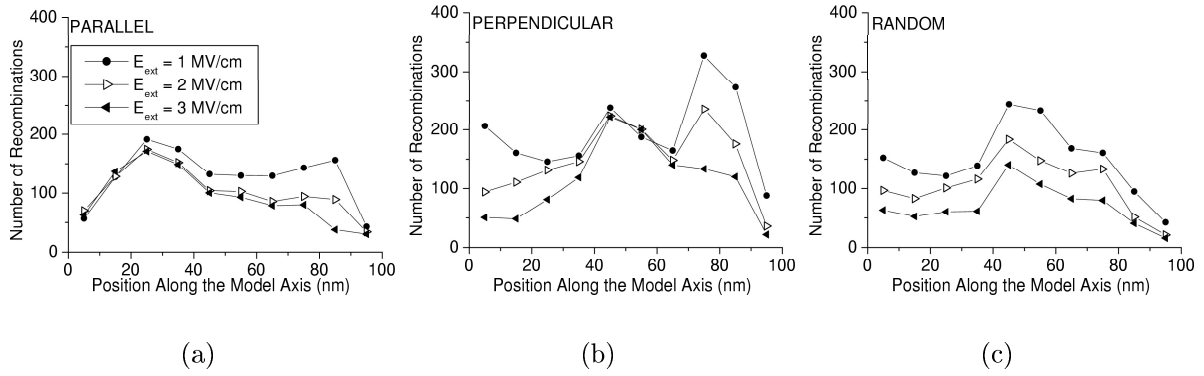


Figure 7. The distribution of recombination events in 8-CN-PPV along the direction perpendicular to the electrode surfaces for three different strengths of the external applied electric field, E_{ext} , and the following chain alignments relative to the electrode surfaces: (a) parallel, (b) perpendicular and (c) random orientation.

for the three molecular arrangements considered in this work and several strengths of the external applied electric field. The behaviour observed for the molecular alignment

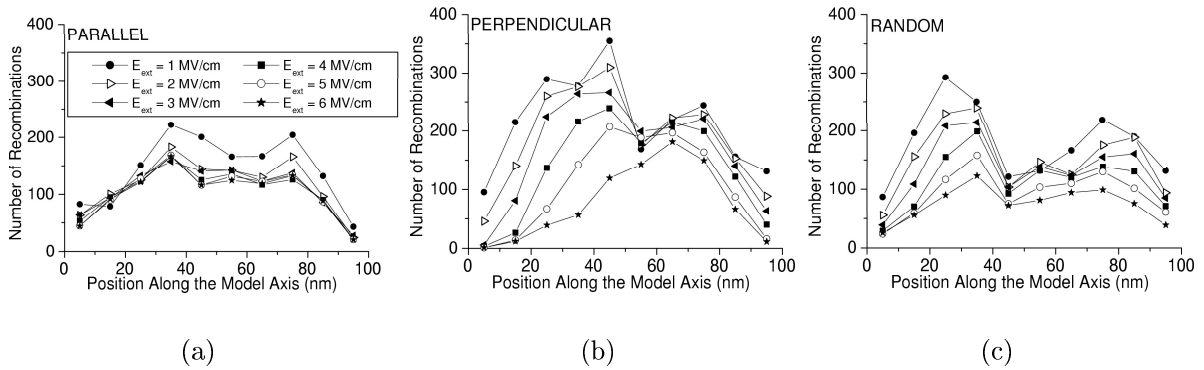


Figure 8. The distribution of recombination events in DMeO-PPV along the direction perpendicular to the electrode surfaces for three different strengths of the external applied electric field, E_{ext} , and the following chain alignments relative to the electrode surfaces: (a) parallel, (b) perpendicular and (c) random orientation.

parallel to the electrode surfaces is similar to what was found for PPV and CN-PPV, since energetic disorder in PPV-based polymers due to changes in conjugation length is similar and charge mobility along the chains does not affect the hopping process. Due to the considerable differences in the local electric field needed for intra-molecular mobility of electrons and holes in DMeO-PPV, the recombination concentrates in this material next to both electrodes for polymer chains either aligned perpendicular to the electrodes or randomly oriented. When the applied field increases, recombinations decrease close

to the electrodes and do not change significantly in the centre of the polymer film. The overall results are the continuous shift of the recombination distribution away from the electrode where the electrons are injected and the change of the recombination profile through the entire layer.

Comparison between figures 7 and 8 also shows that, for all PPV-based polymers, films with chains oriented perpendicular to the electrode surfaces, as those produced by microdroplet deposition [5], have greater recombination efficiency in the centre of the polymer film as compared with parallel orientation for spin-coated films and orientational disorder when high applied fields are used. As a result the film morphology with chain orientation perpendicular to the electrodes should have enhanced luminescence from the array of dipole emitters with sine-square angular distribution of light about the long chain axis.

Based on the above results, we suggest that local molecular packing with high fluorescence efficiency is a plausible explanation for the strong localized variation in luminescence efficiency of a drip coated PPV derivative generated by a scanning tunnelling microscope [25].

4. Conclusions

We have illustrated that generalized Monte Carlo simulations of hopping transport, in which the polymer film morphology and the parameters related to molecular properties are explicitly included, can prove very helpful to assess the influence of molecular arrangements on the properties of light-emitting devices based on PPV and its derivatives. Most importantly, we found that despite the molecular orientation relative to the electrode surfaces has little effect on building-up transient charge trapping within the polymer film, the space-charge due to electrons and holes has surprisingly significant effects on the internal electric field distribution and percolation in charge transport. Our numerical simulations can also give access to a detailed analysis of current and recombination efficiencies. This in turn can be used to gain a theoretical insight into transport and luminescence properties in conjugated polymers with different molecular alignments relative to the electrode surfaces.

Since charge trapping is not significantly affected by the external applied electric field, current efficiency increases. Both current and recombination deviate from linearity at high applied fields for the case of polymer molecules lying with their long axis parallel to the electrode surfaces. This is to be expected as a result of the saturation of the transit time by the electrostatic energy. It was also found that highly oriented polymer films with molecular alignment perpendicular to the electrode surfaces have the highest recombination efficiency in the centre of the film, the effect being less pronounced for polymers with similar electric field threshold for intra-molecular mobility of electrons and holes. On the basis of these theoretical results and the experimental photo-physical properties of conjugated polymer nanoparticles [5], we can conclude that achieving highly uniform oriented films with stiff-chain segments perpendicular to the electrodes

might be a viable strategy for the optimization of the performances of polymer-based LEDs.

Acknowledgments

We would to express our gratitude to Professor Marshall Stoneham for introducing us to the modelling of conjugated polymers and for his continuing support and encouragement. This work was supported by the Portuguese Foundation for Science and Technology (FCT) and the European Community Fund FEDER under the projects number POCTI/CTM/41574/2001 and CONC-REEQ/443/2001. One of us (H.M.G.C.) is also indebted to FCT for financial support under PhD grant n. SFRH/BD/11231/2002.

References

- [1] J. H. Burroughes, D. D. C. Bradley, A. R. Brown, R. N. Marks, K. Mackay, R. H. Friend, P. L. Burns, and A. B. Holmes. Light-emitting-diodes based on conjugated polymers. *Nature*, 347(6293):539–541, 1990.
- [2] M. Redecker, D. D. C. Bradley, M. Inbasekaran, and E. P. Woo. Mobility enhancement through homogeneous nematic alignment of a liquid-crystalline polyfluorene. *Applied Physics Letters*, 74(10):1400–1402, 1999.
- [3] E. J. Samuelsen and J. Mardalen. *Handbook of organic conductive molecules and polymers*, volume 3. Wiley, Chichester, UK, 1997.
- [4] H. Sirringhaus, P. J. Brown, R. H. Friend, M. M. Nielsen, K. Bechgaard, B. M. W. Langeveld-Voss, A. J. H. Spiering, R. A. J. Janssen, E. W. Meijer, P. Herwig, and D. M. de Leeuw. Two-dimensional charge transport in self-organized, high-mobility conjugated polymers. *Nature*, 401(6754):685–688, 1999.
- [5] B. G. Sumpter, P. Kumar, A. Mehta, M. D. Barnes, W. A. Shelton, and R. J. Harrison. Computational study of the structure, dynamics, and photophysical properties of conjugated polymers and oligomers under nanoscale confinement. *Journal of Physical Chemistry B*, 109(16):7671–7685, 2005.
- [6] A. B. Walker, A. Kambili, and S. J. Martin. Electrical transport modelling in organic electroluminescent devices. *Journal of Physics-Condensed Matter*, 14(47):12271–12271, 2002.
- [7] S. J. Martin, A. Kambili, and A. B. Walker. Temperature and field dependence of the mobility of highly ordered conjugated polymer films. *Physical Review B*, 67(16), 2003.
- [8] M. M. D. Ramos and A. M. Stoneham. Mesoscopic modelling of charge evolution in conducting polymers. *Computational Materials Science*, 17(2-4):260–264, 2000.
- [9] M. M. D. Ramos and A. M. Stoneham. Mesoscopic study of bipolar charge transport in polymer-based devices. *Synthetic Metals*, 122(1):149–151, 2001.
- [10] A. M. Stoneham and M. M. D. Ramos. Mesoscopic modelling of conducting and semiconducting polymers. *Journal of Physics-Condensed Matter*, 13(10):2411–2424, 2001.
- [11] A. M. Stoneham, M. M. D. Ramos, A. M. Almeida, H. M. G. Correia, R. M. Ribeiro, H. Ness, and A. J. Fisher. Understanding electron flow in conducting polymer films: injection, mobility, recombination and mesostructure. *Journal of Physics-Condensed Matter*, 14(42):9877–9898, 2002.
- [12] M. M. D. Ramos, A. M. Almeida, H. M. G. Correia, R. M. Ribeiro, and A. M. Stoneham. Effect of molecular properties on the performance of polymer light-emitting diodes. *Applied Surface Science*, 238(1-4):438–443, 2004.
- [13] M. M. D. Ramos, H. M. G. Correia, R. M. Ribeiro, and A. M. Stoneham. Mesoscopic modelling of bipolar charge evolution in CN-PPV LEDs. *Synthetic Metals*, 147(1-3):281–286, 2004.

- [14] T. G. Bjorklund, S. H. Lim, and C. J. Bardeen. Use of picosecond fluorescence dynamics as an indicator of exciton motion in conjugated polymers: Dependence on chemical structure and temperature. *Journal of Physical Chemistry B*, 105(48):11970–11977, 2001.
- [15] D. S. Wallace. *Electron-lattice coupling in conjugated polymers*. PhD thesis, University of Oxford, 1989.
- [16] D. S. Wallace, A. M. Stoneham, W. Hayes, A. J. Fisher, and A. H. Harker. Theory of defects in conducting polymers .1. theoretical principles and simple applications. *Journal of Physics-Condensed Matter*, 3(22):3879–3903, 1991.
- [17] M. M. D. Ramos and A. M. Almeida. Charge-induced defects in poly-phenylene-vinylene (PPV). *Vacuum*, 64(2):99–104, 2001.
- [18] H. M. G. Correia and M. M. D. Ramos. Modeling charge transport properties of cyano-substituted PPV. *Materials Science & Engineering C-Biomimetic and Supramolecular Systems*, 23(6-8):773–777, 2003.
- [19] H. M. G. Correia and M. M. D. Ramos. Intra-molecular properties of DMeOPPV studied by quantum molecular dynamics. *Computational Materials Science*, 33(1-3):218–223, 2005.
- [20] N. Tessler, N. T. Harrison, and R. H. Friend. High peak brightness polymer light-emitting diodes. *Advanced Materials*, 10(1):64–68, 1998.
- [21] J. C. Scott, S. Ramos, and G. G. Malliaras. Transient space-charge-limited current measurements of mobility in a luminescent polymer. *Journal of Imaging Science and Technology*, 43(3):233–236, 1999.
- [22] J. C. Scott, P. J. Brock, J. R. Salem, S. Ramos, G. G. Malliaras, S. A. Carter, and L. Bozano. Charge transport processes in organic light-emitting devices. *Synthetic Metals*, 111:289–293, 2000.
- [23] C. Tanase, P. W. M. Blom, and D. M. de Leeuw. Origin of the enhanced space-charge-limited current in poly(p-phenylene vinylene). *Physical Review B*, 70(19):193202, 2004.
- [24] W. F. Pasveer, J. Cottaar, C. Tanase, R. Coehoorn, P. A. Bobbert, P. W. M. Blom, D. M. de Leeuw, and M. A. J. Michels. Unified description of charge-carrier mobilities in disordered semiconducting polymers. *Physical Review Letters*, 94(20), 2005.
- [25] D. G. Lidzey, S. F. Alvarado, P. F. Seidler, A. Bleyer, and D. D. C. Bradley. Electroluminescence from a soluble poly(p-phenylenevinylene) derivative generated using a scanning tunneling microscope. *Applied Physics Letters*, 71(14):2008–2010, 1997.