

PACS 71.20.Rv, 85.60.Jb

Numerical study of electrical characteristics of conjugated polymer light-emitting diodes

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Abstract. Conjugated polymers now provide a class of processible, film-forming semiconductors and metals. In this work, the electronic properties of polymer light-emitting diodes devices are numerically studied. Our results show how an insulating buffer layer with suitable thickness decreases the barrier height at the cathode and therefore increases the electron injection. We also discuss the effects from persistent charged traps.

Keywords: polymer; light-emitting diode; current density.

Manuscript received 31.10.07; accepted for publication 15.05.08; published online 30.06.08.

1. Introduction

A large amount of attention has been paid to the development of nanotechnology because nanomaterials exhibit special electrical, optical and magnetic properties that differ from those of atoms and bulk. The unique properties of nanomaterials are caused by quantum-confinement or surface effects that become operative on that scale [1].

Conjugated polymers have many advantages in terms of versatile multicolor emission controlled readily by the molecular structure and facile fabrication of small and large area active layers by spin coating or printing technology. Various polymerization methods for the synthesis of electroluminescent (EL) polymers have been developed such as Wittig reaction [2], Heck reaction [3], and Suzuki reaction [4]. Of the fact that the Conjugated polymers derive their semiconducting properties from having delocalized π -electron bonding along the polymer chain. The π bonding and π^* antibonding orbitals form delocalized valence and conduction wave functions, which support mobile charge carriers. The current efficiency is strongly reduced at low voltages. Electroluminescence from conjugated polymers was first reported [5] using poly (phenylenevinylene) (PPV).

In this paper, we numerically review progress that has been made in the use of conjugated copolymers in LEDs.

2. Electronic model

2.1. Fundamental processes

The device operation of a polymer LED is thus determined by three processes: charge injection, charge transport and recombination. An unbalanced charge injection results in an excess of one carrier type and thus in a current flow which practically does not contribute to the light emission. As a result, the presence of a contact barrier which hinders sufficient injection of one type of charge carrier will exhibit a low efficiency. Reduction of the contact barriers leads to a larger current and a higher light-output at an equal voltage. Thus, in order to maximize the PLED efficiency the work function of the cathode and anode should both be close to the conduction and valence bands of the PPV, respectively. Therefore, a low work function metal cathode, such as Ca, and a high work function anode, such as ITO, are preferably used. An unbalanced charge transport also affects the device efficiency of a PLED. A reduced electron transport with regard to the hole transport, for example due to the presence of electron traps, would give rise to confinement of the electroluminescence in a region close to the cathode. Since metallic electrodes are very efficient quenching centers for the generated EL such a confinement would strongly decrease the device performance. Finally, the recombination process of electrons and holes in the active polymer layer directly determines the light-output and thus the efficiency of the PLED.

2.2. Device model

Several electronic models of PLEDs have been proposed in the past few years [6-8] In this work, the equations of one-dimensional time-independent PLED model that governs the electrical behavior are as follows [9-13]

$$\frac{dJ_n}{dx} = qr(x)p(x)n(x), \quad (1)$$

$$\frac{dJ_p}{dx} = -qr(x)p(x)n(x), \quad (2)$$

$$\frac{dE(x)}{dx} = \frac{q}{\epsilon_s \epsilon_0} (p(x) - n(x)). \quad (3)$$

Here, n is the density of electrons, p is the density of holes, E is the electric field, ϵ_0 is the vacuum permittivity, ϵ_s is the relative permittivity, q is the electron charge magnitude, and r is the Langevin recombination rate coefficient. The effective voltage is equal to the applied voltage minus the built-in potential

$$V_{\text{eff}} = V_{\text{app}} - V_{\text{bi}} = \int_0^L E(x) dx. \quad (4)$$

The electron current density and hole current density can be written as [8]

$$J_n = q\mu_n(x, E)n(x)E(x) + qD_n(\mu_n)\frac{dn(x)}{dx}, \quad (5)$$

$$J_p = q\mu_p(x, E)p(x)E(x) - qD_p(\mu_p)\frac{dp(x)}{dx}, \quad (6)$$

where μ_n and μ_p are the electron and hole mobilities, and D_n and D_p are the electron and hole diffusion coefficients related to the charge mobility by the Einstein relation $qD = \mu k_B T$.

3. Structure and materials

The structural diagram and the organic materials of the PLED device under study are shown in Fig. 1.

In this structure, the indium-tin oxide (ITO) layer functions as a transparent electrode and allows the light generated within the diode to leave the device. The top electrode is conveniently formed by thermal evaporation of a metal. LED operation is achieved when the diode is biased sufficiently to achieve injection of positive and negative charge carriers from opposite electrodes. Capture of oppositely charged carriers within the region of the polymer layer can then result in photon emission. The chemical structures of polymers used here are shown in Fig. 2.

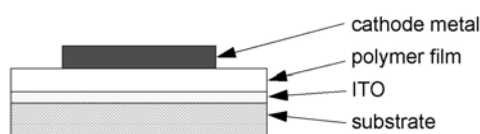


Fig. 1. Structure of a single layer polymer light-emitting device.

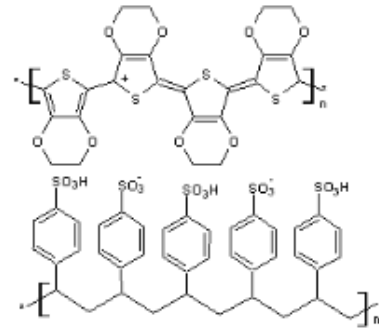


Fig. 2. Chemical structure of polymer poly (3,4-ethylenedioxythiophene) poly-(styrenesulfonate) PEDOT-PSS.

Conjugated polymer – PEDOT has unique combination of properties which makes it extremely attractive for organic electronics applications. It is utilized in organic-based optoelectronic devices: as a charge injecting layer in light emitting devices; as a component in electrochromic displays and even as electrodes in field effect transistors and photovoltaic cells. PEDOT is an intrinsically insoluble polymer, which can be chemically or electrochemically doped. Doping transforms PEDOT from an opaque insulator to a quasi-transparent material with high electrical conductivity. The most common form, in which PEDOT is used, comprises poly(styrenesulfonate) abbreviated often as PSS. The distinct property of such complex, known as PEDOT-PSS, is its solubility in water. The synthesis of PEDOT-PSS involves polymerization of EDOT monomers in a polyelectrolyte solution of PSS. Polymerization is initiated by removal of charges from EDOT monomers. Formed in this way radicals promote polymerization of EDOT units while PSS acts as counter ion balancing positive charge residing on PEDOT. The final product comprises of aqueous dispersion of PEDOT-PSS. PEDOT chain stores charges in the form of polarons/bipolarons.

4. Simulation results and discussion

In Fig. 3, the current density as a function of the drive voltage in the forward bias are shown for a single-layer ITO / PEDOT:PSS / Al device with a layer thickness of 85 nm. Forward bias is defined as the positive voltage on the hole-injecting ITO contact. The LEDs with PEDOT:PSS as active layer (100 nm) started emitting light at a turn-on voltage of 1.5 V. This corresponds to an electric field strength ($E = V/d$, d is the layer thickness) at turn-on of 1.610^6 V/m. Turn-on voltage is defined here as the voltage at which the electroluminescence starts exceeding the background signal.

The modified “current density – voltage” characteristic at a proper thickness of the buffer layer is shown in Fig. 4. When a buffer layer with proper thickness is introduced, the current density of electrons is larger than that of a buffer-free device at the same voltage, which attributes to the improved electron injection.

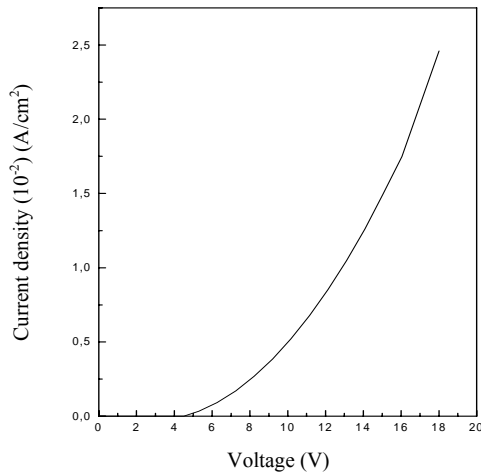


Fig. 3. Current density as a function of the voltage for an ITO/PEDOT:PSS.

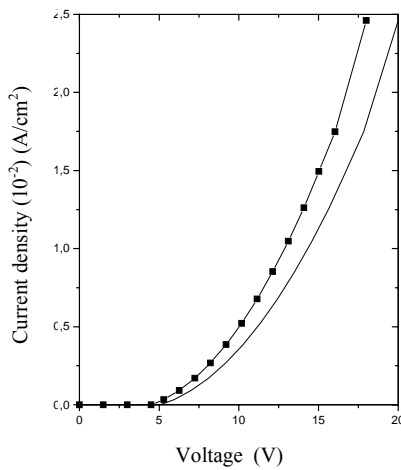


Fig. 4. Current density as a function of the voltage using BaO/Al or Al as a cathode.

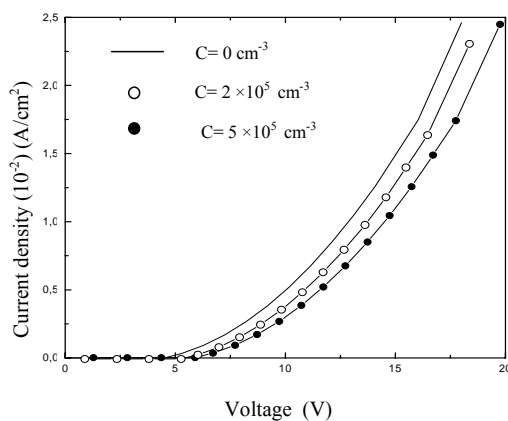


Fig. 5. Current density as a function of the voltage for different values of trap concentrations.

We show how trapped charges affect the characteristics devices. This effect of traps can be incorporated by an additional term in Eq. (3)

$$\frac{dE(x)}{dx} = \frac{e}{\epsilon_s \epsilon_0} [p(x) - n(x) \pm n_t(x)]. \quad (7)$$

We considered that electron traps with a density C in the range of 10^{15} cm^{-3} located at the cathode side with a step distribution function $n_t(x) = C$. In Fig. 5, we show if the device is operated at a constant current, the operation voltage increases and efficiency decreases as electrons are being trapped and accumulated.

5. Conclusion

In summary, we have investigated the origin of the bias dependence of the current in a polymer light-emitting diode based on a single active layer of poly (3,4-ethylenedioxythiophene)poly-(styrenesulfonate). We successfully proved that the electron injection increases by introducing an insulating buffer layer. The effects of persistent charged traps were easily incorporated into the calculation. These results revealed that voltage increase observed during constant current operation, which is one of the significant degradation processes in real devices, may be caused by the accumulation of electrons in the vicinity of the cathode.

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