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Modeling and numerical study of electrical characteristics of polymer light-emitting diodes containing an insulating buffer layer

Dexi Zhu *, Hui Ye, Jun Gao, Xu Liu

State key laboratory of Modern Optical Instrumentation, Zhejiang University, Hangzhou 310027, PR China

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Abstract

In order to improve the electrical characteristic of polymer light-emitting diodes, a simple model for the device characteristic with an insulating buffer layer at cathode is proposed. This model is based on Fowleer–Nordhein tunneling mechanism and Poission's equation. An additional tunneling factor which characterises the tunneling effect of buffer layer is introduced. The simulated current–voltage characteristic indicates how an insulating buffer layer with suitable thickness decreases the barrier height at the cathode and therefore increases the electron injection. The model is validated by experimental results of devices with BaO as the buffer material and poly[2-methoxy-5-(2′-ethyl-hexyloxy)-1,4-phenylenevinylene] as the emission material. An optimum thickness of the buffer layer is also obtained from the model, which provides a guide to device design.
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Keywords: Polymer light-emitting diodes; Model; Insulating buffer layer; Electrical characteristics

1. Introduction

Polymer light-emitting diodes (PLEDs) have been attracting much attention recently as a technology for full-color displays. The electroluminescence from PLEDs is caused through relaxing of excitons which are formed by carrier injection from the anode and cathode. By the study of the basic principles of electroluminescence of PLEDs, it is found that the balance between the hole and electron concentrations has a crucial influence upon the electrical characteristics, such as drive voltage and efficiency of luminescence. In addition, most emissive polymeric materials act as hole transporters, and are found poor in electron transport. For example, hole mobility of poly[2-methoxy-5-(2′-ethyl-hexyloxy)-1,4-phenylenevinylene] (MEH-PPV) is about ten times larger than that of electron. For this reason, it's helpful to improve the electron injection from the cathode for the purpose of achieving better electrical and optical properties for PLEDs [1].

Many efforts have been made to improve the electron injection. Among them proper insertion of a thin buffer layer between the cathode and the polymer layer has been reported [2]. Usually, the materials used as the buffer layer are insulators, such as alkali–halide [3] or oxide [4]. In contrast to the conventional view that an extra insulating layer might increase the turn-on voltage, the fact is that the turn-on voltage decreases and quantum efficiency increases when a buffer layer is introduced [5]. Park et al. proposed that the mechanism of the enhanced electron injection originated from a lowering of the barrier height between the cathode and emission layer [6]. The energy level diagram is shown in Fig. 1, where 1, 2, 3 and 4 are the anode (or hole-injecting layer), the polymer layer, the cathode and the buffer layer, respectively. E_f is the cathode Fermi level. LUMO means polymer lowest unoccupied molecular orbital while HOMO means highest occupied molecular orbital. If no buffer layer is inserted, the electron must tunnel through the barrier from the E_f to LUMO as shown in the left diagram. When a buffer layer with proper thickness is introduced as shown in the right diagram, the forward voltage drops across the insulating layer is ΔV. So the barrier will be $e\Delta V$ smaller than that in the buffer-free case, resulting in an increased injection current.

* Corresponding author. Tel.: +86 571 87951190; fax: +86 571 87951758.
E-mail address: zhudexioo@hotmail.com (D. Zhu).

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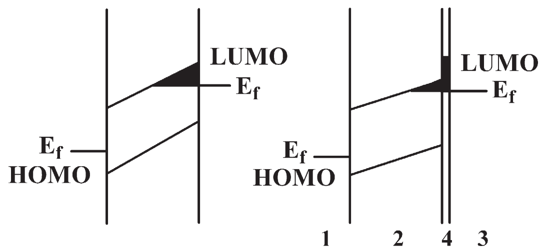

Fig. 1. A sample model of energy level diagram of PLEDs with different cathodes.

In general, device model provides a useful tool for facilitating device design. Some numerical models have been reported. Y. Kawabe et al. [7] proposed a model for single layer devices in which the current density–voltage (*J–V*) characteristics were obtained numerically. It showed that the current depends on the barrier height at the metal-organic interface. However, the additional insulating layer was ignored in this model, which was therefore unsuitable for bilayer-cathode devices. In this paper, we propose a simple model for simulating the device characteristics of PLEDs containing insulating buffer layers with different thickness. This model is based on Poisson's equation and Fowleer–Nordhein (FN) tunneling mechanism. A tunneling factor is introduced to take the effect of the insulating buffer layer into consideration. The current densities are simulated for different thicknesses of buffer layers and the optimum thickness is obtained for a certain material, which is in agreement with the experimental result.

2. The model

For the research of the effect of a buffer layer on the carrier injection, the interfaces between emission layer and two electrodes are significant. So double-carrier injection is considered in our model. Meanwhile, we assume that the injection is driven by FN tunneling mechanism [8] which shows the relationship between current and potential barrier height at two interfaces. We define the coordinate that the anode position is at $x=0$, and the cathode one is at $x=d$. The current density can be expressed by the following equation:

$$J_0 = \mathrm{FN}(E) = k_1 \frac{E^2}{\Phi} \exp\left(-k_2 \frac{\Phi^{3/2}}{E}\right)$$

$$k_1 = \frac{2.2e^2}{8\pi h}$$

$$k_2 = \frac{8\pi}{3h}(2em^*)^{1/2} \tag{1}$$

where e is the elementary charge, h is Planck's constant, m^* is the effective mass of an electron or a hole (for simplicity, $m^*=m_0$ herewith), Φ is the potential barrier height, and E is the electric field at the interface where the carriers are injected.

We assume that the carrier density in emission layer is not uniform. That means the carrier density is the largest at the interface between electrode and emission layer and declines exponentially inside. This is analogous to the diffusion of minority carriers in the active layer of semiconductor. Therefore, the densities of holes and electrons can be expressed as following [9]:

$$p(x) = p_0 \exp(-x/r_0) \tag{2.a}$$

$$n(x) = n_0 \exp((x-d)/r_0) \tag{2.b}$$

where x is the coordinate normal to the device. $x=0$ corresponds to the interface position of anode and emission layer. p and n are the densities of holes and electrons, respectively. r_0 is the characteristic length characterising the distribution of carriers in the emission layer. p_0 and n_0 are the largest densities in the device. We assume that the current densities caused by holes and electrons are constant throughout the device, given by:

$$J_h(x) = J_h = E_0 p_0 \mu_h e \tag{3.a}$$

$$J_e(x) = J_e = E_d n_0 \mu_e e \tag{3.b}$$

where subscripts h and e refer to holes and electrons, respectively. μ is the carrier mobility, E_d is the electric field at $x=d$. The electric field and carrier density are related through Poisson's equation:

$$\frac{\mathrm{d}E(x)}{\mathrm{d}x} = \frac{e}{\varepsilon}\{p(x) - n(x)\}. \tag{4}$$

Where ε is the dielectric constant of the polymer layer. By integrating Eq. (4) and combining it with Eqs. (2.a) and (2.b), we get the electric field distribution:

$$E(x) = E_0 + \frac{ep_0r_0}{\varepsilon}\left[1 - \exp\left(-\frac{x}{r_0}\right)\right] - \frac{en_0r_0}{\varepsilon}\left[\exp\left(\frac{x-d}{r_0}\right) - \exp\left(-\frac{d}{r_0}\right)\right]. \tag{5}$$

Where $p_0 = \frac{\mathrm{FN}(E_0)}{\mathrm{E}_0\mu_h e}$, $n_0 = \frac{\mathrm{FN}(E_d)}{E_d\mu_e e}$ according to Eqs. (1), (3.a), and (3.b). So we can get E_d at $x=d$. The voltage can be derived by integrating Eq. (5):

$$V = E_0 d + \frac{ep_0r_0}{\varepsilon}\left\{r_0\left[\exp\left(-\frac{d}{r_0}\right) - 1\right] + d\right\} - \frac{en_0r_0}{\varepsilon}\left\{r_0\left[1 - \exp\left(-\frac{d}{r_0}\right)\right] - d\exp\left(-\frac{d}{r_0}\right)\right\}. \tag{6}$$

The total current density is the sum of current densities of electrons and holes:

$$J_{\mathrm{total}}(E_0) = J_h + J_e. \tag{7}$$

Where J_h and J_e are both in the form of Eq. (1), which is a function of electric field E_0 when other parameters are known. Eq. (6) shows the voltage V is also a function of E_0. It means all equations can be determined when E_0 is chosen. Therefore, the *J–V* characteristic can be plotted according to Eqs. (6) and (7). Fig. 2 shows the simulated *J–V* curve based on the buffer-free

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