Effect of field dependent trap occupancy on current conduction in single layer organic light-emitting devices including both bulk and injection effects

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A model to calculate the current density-voltage characteristics for single carrier organic polymers taking into account the influence of high electric field on trap occupancy is presented. The case of the traps with exponential distribution in energy is considered in detail. The field dependent trap occupancy model is found to change the electric field distribution and J-V characteristics of the organic layer significantly. The model is compared with the experimental data obtained by A. L. Alvarez et al. [15]. There is good agreement between experimental data and our model.

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1. Introduction

Recently there has been considerable interest in organic light-emitting devices (OLEDs) [1-6]. Current density-voltage characteristics (J-V) are often modeled assuming either only the bulk effect or only the injection effect. However, in most practical devices, the current is limited by both the bulk effect and the injection effect when a moderate barrier for carrier injection is present, e.g., 0.2-0.5 eV. The model of thermally assisted tunneling proposed by M. A. Abkowitz et al. [7] can calculate the J-V characteristics in such devices but the effect of traps is not taken into account explicitly. It has been shown that traps play an important role in determining the J–V characteristics of organic semiconductors [8]. Though Y.Q. Peng et al. [9] have investigated the effect of traps on the J –V curves, field dependent occupancy of traps [10] was not considered. V. Kumar et al. [10] have shown that the effect of electric field on the ionization energy of the traps (Poole–Frenkel like effect) is necessary to interpret the experiments on organic polymers, which was not taken into account by Y.Q. Peng et al. [9] It is therefore necessary to re-examine the effect of traps on the performance characteristics of an OLED taking into account the effect of high electric fields on the occupancy of the traps. The purpose of this article is to investigate the effect of field dependent trap occupancy (FDTO) on the OLEDs characteristics. Our basic approach is essentially the same as that of Y.Q. Peng et al. [9] for the effects of traps and as that of V. Kumar et al. [10] for the FDTO.

2. Model

It is useful to consider an organic polymer structure in which a single carrier-type (i.e., either electrons or holes) dominates the current flow in order to clarify the device operation in a relatively simple situation [11]. The following discussions are based on single layer OLEDs made of hole transport organic electroluminescent materials, but the results are also valid for OLEDs made of electron transport materials, when the charge, density and mobility of holes are replaced by that of electrons.

In the absence of FDTO, the characteristics of single carrier devices are calculated using the following equations:

$$\frac{dF(x)}{dx} = \frac{q(p_f + p_t)}{\varepsilon_0 \varepsilon_r}, \tag{1}$$

$$J_b = q\mu p_f F(x), \tag{2}$$

along with the boundary condition,

$$U = \int_0^d F(x)dx. \tag{3}$$

Here, $F(x)$ is the field, d is the sample thickness, q is the charge of holes, ε_0 and ε_r are the permittivity of vacuum and the relative dielectric constant of organic materials, respectively, p_f and p_t are free hole and trapped hole density, respectively, μ is the hole mobility, J_b is the total current in the organic bulk. The zero point of coordinate x is located at the interface between the anode and the organic layer. According to TCL theory, the trap density in an organic layer is distributed in energy as follows [12]:

$$h(E) = \frac{H_b}{kT_c}\exp\left(\frac{-E}{kT_c}\right), \tag{4}$$

where E is the energy of traps respective to the energy of the highest occupied molecular orbit (HOMO), H_b is the density of traps states per unit energy in the vicinity of energy E , T_c is a characteristic constant of the distribution and k is the Boltzmann constant. The concentration of trapped holes is [10]

$$p_t = \alpha H_b (p_f / N_v)^{1/l}, \tag{5}$$

where $l = T_c / T$, $\alpha = (\pi / l) / \sin(\pi / l)$, T is the temperature, N_v is the effective density of states in the valence band.

According to the Fowler–Nordheim tunnel theory, the electric current from the injection electrode can be interpreted as follows: [13]

$$J_{inj} = \frac{c}{\phi} F_0{}^2 e^{\frac{-B\phi^{3/2}}{F_0}}, \tag{6}$$

where $c = \dfrac{2.2q^3}{8\pi h}$, $B = \dfrac{8\pi\sqrt{2m^*}}{2.96hq}$.

Here ϕ and F_0 denote the barrier height and the electric field at the carrier injection electrode, respectively, and m^* and h are effective carrier mass and Plank constant, respectively. From the principle of current continuality, we have

$$J_b = J_{inj}. \tag{7}$$

To obtain the current density-voltage characteristics (J-V) we can solve numerically the equations (1)–(7).

We now modify the above equations to take into account the effect of high field on trap occupancy. [10] The trapped carrier concentration is reduced due to the change in the trap ionization energy in the presence of high electric field. The actual reduction in the ionization energy is $B_{eff}\sqrt{F}$ (effective Poole–Frenkel coefficient, see Ref. 10 and the references given therein), where

$$\beta_{eff} = \beta_{PF}\left(\frac{F}{F + \dfrac{q^3 N_t}{8\pi(\varepsilon_r \varepsilon_0)^2 kT}}\right), \tag{8}$$

N_t is the trap density (per cm^3) and β_{PF} [8] is given by

$$\beta_{PF} = \left(\frac{q^3}{\pi \varepsilon_r \varepsilon_0}\right)^{1/2}. \tag{9}$$

In the presence of FDTO, Eq. (5) changes to [10]

$$p_t = \alpha H_b \exp[(-\beta_{eff}\sqrt{F}) / kT_c](p_f / N_v)^{1/l}. \tag{10}$$

It is seen from Eq. (10) that the calculation of the trapped carrier density p_t requires electric field F when the field effect is switched on. To obtain the new current density-voltage characteristics we can also solve numerically equations (1), (2), (3), (4), (6), (7), (8), (9), (10).

3. Results and discussion

The distribution of the electric field in the organic layer is shown in Figs. 1 and 2. The solid lines show the electric field calculated with the FDTO model and the dashed lines, without the field effect on trap occupancy. For a given barrier height, the slopes of the field distribution with and without FDTO are quasi- equal for the low operation voltages but the slopes are considerably reduced when the effect of field on trap occupancy is taken into account for the high operation voltages (Fig. 1). This result is consistent with the fact that with FDTO the field modifies the trap carrier density substantially. The direct effect of the FDTO model is to increase the number of free carriers and decrease the trapped carriers [10]. It is easy to see that at the same distance to the anode, the electric field increases with the operation voltages for a given barrier height (Fig. 1). The trapped hole concentration p_t is reduced due to the decrease in the trap ionization energy under high field, thus lowering carrier accumulation and the bulk effect. For a given bias, the slopes of the field distribution with and without FDTO are quasi- equal for the large barrier height at the anode, and is expected to be zero, but as the barrier height decreases the slopes are considerably reduced when the effect of field on trap occupancy is taken into account (Fig. 2). This is because as the barrier height decreases, the number of injected carriers and the trapped and free charges in the organic bulk increase sharply, so the field distribution tends to be non-uniform, which is just the character of bulk limited conduction. At a sufficiently high injection rate, all traps are filled, and the current through the organics attains space-charge-limited current characteristics [10, 14]. V. Kumar et al. [10] show that the effect of electric field on the trap occupancy is very large in space-charge-limited conduction.

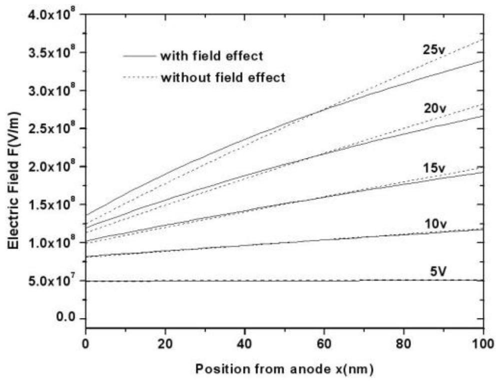

Fig. 1. The distribution of the electric field in the organic layer for different operation voltages with the parameters ϕ =0.5eV, d =100 nm, T =300 K, T_C = 1700K μ =2.6×$10^{-9}m^2V^{-1}s^{-1}$, N_v =5×$10^{19}cm^{-3}$, H_b =1 5×$10^{18}cm^{-3}$, N_t =2×10^{19} $cm^{-3}$and ε_r = 2.

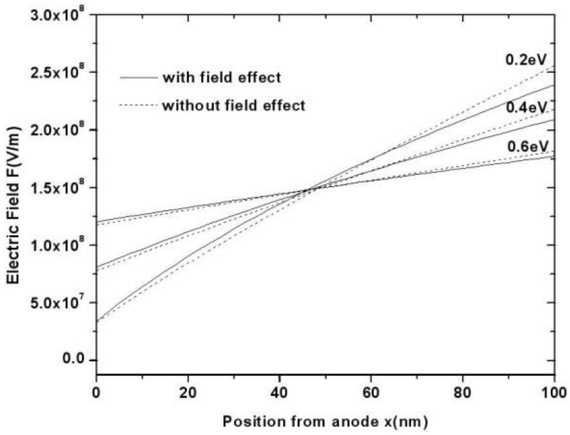

Fig. 2. The distribution of the electric field for different barrier heights. The parameters used are d =100 nm, T =300 K, T_C =1700 K, μ =2.6×10^{-9}m^{2}V^{-1} s^{-1}, N_v =5×10^{19}cm^{-3}, H_b =1.5×10^{18}cm^{-3} , N_t =2×10^{19} cm^{-3}, ε_r = 2 and U =15V.

Figs. 3 and 4 show the numerically calculated J -V curves. The solid lines show the current density calculated with the FDTO model and the dash lines, without the field effect on trap occupancy. For a given thickness and operation voltage, the current density with FDTO is larger than that without FDTO (Figs. 3). The field effect increases the current density by a few orders of magnitude. Fig. 4 shows that for a given operation voltage and barrier height at the anode, the current density is also considerably increased when effect of field on trap occupancy is taken into account.

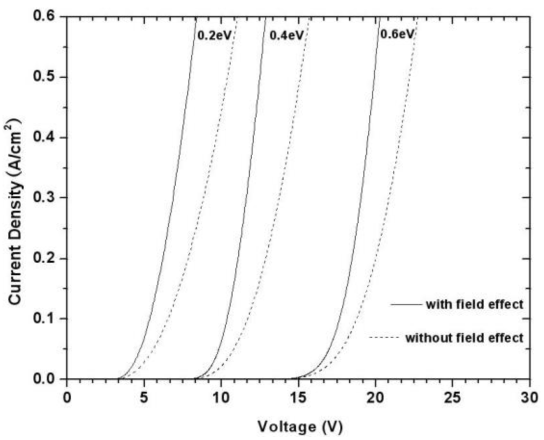

Fig. 3. The current density–voltage characteristics for different injection barrier heights with the parameters d = 100 nm, T = 300 K, T_C = 600 K, μ = 5×10^{-9}m^{2}V^{-1}s^{-1}, N_v =1.2×10^{19}cm^{-3}, H_b =1×10^{18}cm^{-3}, N_t =4×10^{18}cm^{-3}, and ε_r = 3 .

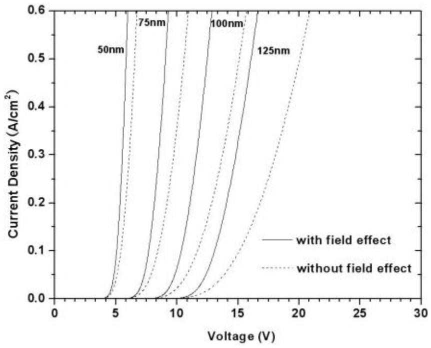

Fig. 4. The current density–voltage characteristics for different thickness of the organic layer with the parameters ϕ = 0.4 eV, T = 300 K, T_C = 600 K, μ=5×10^{-9}m^{2}V^{-1}s^{-1}, N_v=1.2×10^{19}cm^{-3}, H_b =1×10^{18}cm^{-3}, N_t =4×10^{18}cm^{-3}, and ε_r = 3 .

We have compared the experimental J-V characteristics of A.L. Alvarez et al. [15] for hole only ITO/PEDOT: PSS/MDMO-PPV/Al structure with the FDTO model. Poly (2-methoxy-5-{3', 7'-dimethyloctyloxy}- p -phenylenevinylene) (MDMO-PPV) is known as a hole-conducting polymer with a mobility of about 8.3×10^{-10}m^{2}V^{-1}s^{-1} [15]. Its HOMO is about 5.3 eV, 0.5 eV higher than that of ITO [16]. The single layer device with the structure ITO/PEDOT: PSS/MDMO-PPV/Al has a hole-injection barrier of 0.5 eV at the anode. The experimental J-V characteristic of the MDMO-PPV sample (d =60 nm) is shown by symbols in Fig. 5. A solid line shows the current density calculated using our FDTO model with exponentially distributed traps and a dashed line, without the field effect on trap occupancy. The parameters used in calculations are T_C =600 K, H_b =3.1×10^{19}cm^{-3}, N_t = 1.8 ×10^{20}cm^{-3}, N_v =5.1×10^{20}cm^{-3}, μ =8.3×10^{-10}m^{2}V^{-1}s^{-1}, and $\varepsilon_r = 4\varepsilon_0$. Fig. 5 shows that the agreement between the experimental data and our model is excellent.

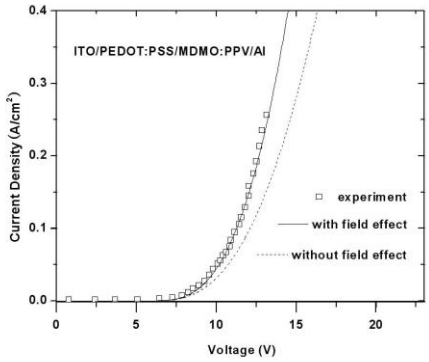

Fig. 5. The simulation and experiment of the current density–voltage characteristics for the ITO/PEDOT: PSS/MDMO-PPV/Al device with thickness of 60 nm. The fit parameters are ϕ = 0.5 eV, T=300 K, T_C=600 K, μ = 8.3×10^{-10}m^{2}V^{-1}s^{-1}, N_v =5.1×10^{20} cm^{-3}, H_b = 3.1×10^{19}cm^{-3}, N_t = 1.8 × 10^{20} cm^{-3}, ε_r = 4, and the data of the experiment are from [15].

4. Conclusions

It is known that traps modify the characteristics of an organic semiconductor considerably [8]. Recently it has been shown that the effect of high electric field (commonly known as the Poole–Frenkel effect) on the ionization energy of the traps changes considerably the free carrier density and J-V characteristics of polymer diodes [10]. We have presented a new model of carrier transport in single layer OLEDs including both bulk and injection effects. The model takes into account the field dependent occupancy of traps. The numerical calculations show that in the practical cases the FDTO modifies the transport characteristics significantly. We have compared our model with the experimental data obtained by A. L. Alvarez et al. [15]. The agreement between the model calculations and the experimental results is very good.

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