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Numerical Device Model and Determination of Device Parameters for Organic Light Emitting Diodes (OLEDs)

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We propose a novel Schottky and impedance spectroscopy (IS) numerical model to evaluate carrier injection and transport behaviour of organic semiconductor materials. Using temperature dependent current-voltage (I-V) and IS measurements of hole only (HOD), electron only (EOD) devices and OLEDs, we have obtained values for the Richardson factor, the barrier height, trap density, density of states (DOS) and carrier mobility of organic materials and interfaces as device parameters.

1. Introduction

Recently, organic light emitting diodes (OLED) have made significant progress in brightness and lifetime to the extent that they now present themselves as a viable technology for application in large-area flat panel displays (FPD) to compete with liquid crystal display (LCD) and plasma technologies. However, the operating mechanisms such as charge-injection, -transport, -trapping, and -recombination phenomena in organic semiconductors are still unclear and require further investigation.

A common approach to estimate the barrier height of an organic-conductor interface is to apply the Richardson-Schottky model [1] with the value of the Richardson Factor (A^*) set for a silicon-metal interface. Alternatively, Scott [2] has proposed that the value of A^* for an organic-conductor interface is dependent on the state density and carrier mobility of the organic material.

Several other groups have reported experimental and measurement methods for extraction of device parameters such as carrier mobility, density of states (DOS) and barrier height [3]. Impedance spectroscopy (IS) has been shown to be a useful tool for evaluating relaxation, transport and injection in a variety of organic devices [4-5].

In this paper, we propose a novel Schottky and IS numerical model to evaluate carrier injection and transport behaviour of organic semiconductor materials. We have obtained values for A^*, the barrier height, interface state density, DOS and carrier mobility of organic materials and interfaces as device parameters.

2. Theory

2.1. Modified Schottky model

The current density of a Schottky organic-conductor interface is expressed as

$$J_{inj} = A^* T^2 exp\left(\frac{-e\left(\phi_B - \sqrt{eE/4\pi\varepsilon_i}\right)}{k_B T}\right) \tag{1}$$

$$A^* = \frac{16\pi\varepsilon\varepsilon_0 N_0 \mu k_B^{\ 2}}{e^2} \quad [A/cm^2 K^2] \tag{2}$$

where, A^*, T, e, ϕ_B, E, ε_0, ε, k_B, N_0, and μ are the Richardson factor, temperature, electron charge, barrier height, applied electric field, permittivity of vacuum, relative permittivity, Boltzmann constant, state density and carrier mobility, respectively. The value for A^* as proposed by Scott [1] is dependent on N_0 and μ of the organic material. We have modified the Schottky equation to include ϕ_B and a non-zero electric field.

2.2. Complex capacitance model for impedance spectroscopy (IS)

Complex permittivity and capacitance are described according to

$$\varepsilon_c = \varepsilon_r - i\varepsilon_i \qquad \begin{cases} C_R = \varepsilon_r \dfrac{S}{d} \\ C_I = \varepsilon_i \dfrac{S}{d} = \dfrac{\sigma S}{\omega d} \end{cases}$$

where, C_R, C_I, ε_r, ε_i, σ, ω, S, and d are real part of capacitance, imaginary part of capacitance, real part of permittivity, imaginary part of permittivity, conductance, angular frequency, active area and thickness of organic semiconductor, respectively. C_R and C_I are expressed by Naito's model and our model as follows:

$$C_R(\omega) = \frac{1}{2R_j\delta\omega}\frac{B}{(1+A)^2+B^2} \tag{3}$$

$$C_I(\omega) = \frac{S D_{it}}{2\omega d\,\delta}\nu_{th} S_t C_0 V \exp\left(\frac{-q\left(\phi_B - \sqrt{qE/4\pi\varepsilon_i}\right)}{k_B T}\right)\ln\left(1+\omega^2\tau^2\right) \tag{4}$$

where, R_i, δ, ν_{th}, S_t, C_0, V, q, D_{it}, τ are the low-frequency incremental resistance of the diode, the trapping parameter, the thermal carrier velocity, the capture cross-section, the static electric capacitance of the organic layer, the bias voltage, the electron charge, the interface state density and the time constant for the characteristic time required to fill and empty the interface state, respectively.

The variables A and B are expressed as follows:

$$A = N_t(E_0) S_t \nu_{th} \frac{k_B T\pi}{2\omega}$$

$$\frac{d(\omega B)}{d\omega} = N_t(E_0) S_t \nu_{th} \frac{k_B T\pi}{\omega}$$

$$N_t(E_0) = N_0 \exp\left(-\frac{T_0}{T}\ln\frac{N_V S_t \nu_{th}}{\omega}\right)$$

where, $N_t(E_0)$ is energy distribution of the localized state density at the valence band edge, N_V is effective density of state in the valence band and N_0 is the density of localized states at the valence band edge (DOS).

3. Experimental

3.1. HOD and EOD

We fabricated a hole-only device (HOD) with the structure: glass / ITO (150nm) / TcTa (70nm) / Al (150nm) and an electron-only device (EOD) with the structure: glass / ITO (150nm) / TmPyPB (70nm) /LiF (1nm) / Al (150nm). Temperature dependent I-V characteristics were obtained, under vacuum (1×10^{-2} Pa), with a temperature controlled probe system in order to estimate ϕ_B and A^*. Carrier mobility was calculated using the dark injection (DI) – space charge limited current (SCLC) method [6]. A Solartron SI-1255 & 1296 frequency response analyzer system was used for IS measurements.

3.2. Phosphorescent blue OLED

We also fabricated a standard phosphorescent blue OLED with structure: glass / ITO (150nm) / TcTa (70nm) / mCP:FIrpic (6%,40nm) / TmPyPB (40nm) / LiF (1nm) / Al (150nm). Luminescence and I-V characteristics were obtained with a luminescence colour meter (Topcon MB-7A) and a source-measure unit (Keithley 2400).

4. Results and discussion

4.1 Determination of device parameters for HOD and EOD

The temperature dependent I-V characteristics of the HOD are shown in the Schottky and Arrhenius plots of Fig. 1. From this data and fits to the numerical model, we have estimated ϕ_B(H) = 0.33 eV and A^*(H) = 1.0×10^{-3} A/cm^2/K^2 for the injection of hole carriers (as indicated by the argument "H"). The A^* value of the ITO/TcTa interface is much smaller than for a metal/Si interface [7]. This suggests that A* is strongly dependent on the combination of materials and the interface conditions.

Fig. 2 shows the result of IS measurements and fits to the numerical model. We have estimated D_{it}(H) = 5.0×10^8 /cm^2 and H_0(H) = 1.0×10^{16} /cm^{3}eV for the hole injection side. However, at low frequencies (<10 Hz), the real part of capacitance becomes unstable. We believe that the hole injection interface has a slow trap-and-release phenomenon.

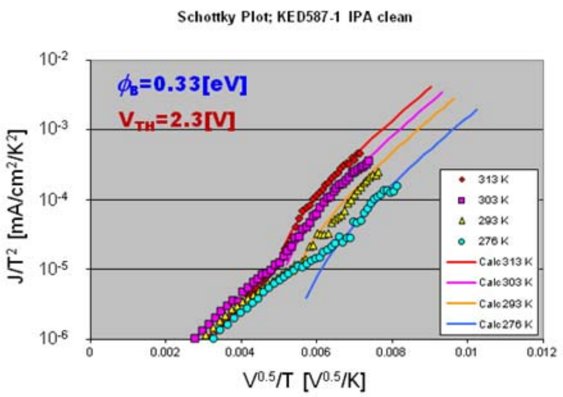

Fig.1(a). Schottky plot of HOD; Glass/ITO(150nm)/ / TcTa (70nm)/Al(150nm) and numerical model fittings. Estimated barrier height f_B for injecting hole is 0.33 eV.

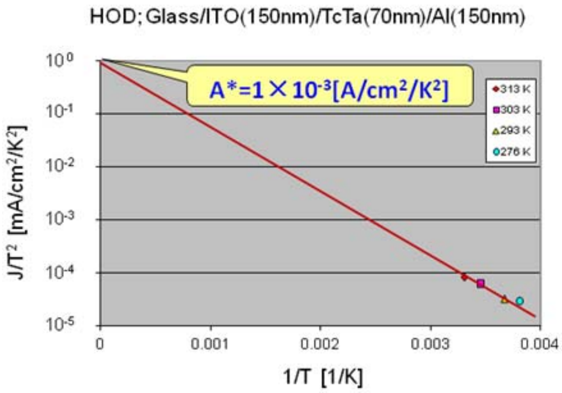

Fig.1(b). Arrhenius plot of HOD; Glass/ITO(150) TcTa(70nm)/Al(150nm). Estimated Richardson factor A* for injecting hole is 1×10^{-3} A/cm^2/K^2 at 0.4 MV/cm.

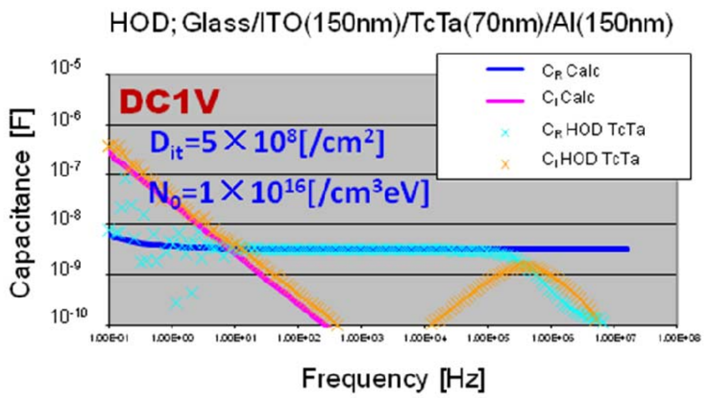

Fig.2. Impedance spectroscopy measurement and model fittings of HOD: Glass/ITO(150nm)/TcTa(70nm)/Al(150nm). Estimated interface state density and density of state (DOS) are 5×10^8 /cm^2 and 1×10^{16} /cm^{3}eV at sub-V_{TH} region, respectively.

Likewise, we also obtained the device parameters for the electron injection interface from the temperature dependent I-V characteristics of the EOD. From the measurement data and fits to the numerical model we have estimated ϕ_B(E) = 0.65 eV, A*(E) = 1.0×10^2 A/cm^2/K^2, D_{it}(E) = 5.0×10^{11} /cm^2 and H_0(E) = 2.0×10^{18} /cm^{3}eV (where the argument "E" is used to indicate electron injection). Our methodologies are an effective means for characterization and determination of the device parameters of single-layer organic devices.

4.2. Characterization of phosphorescent blue OLED

We also obtained the I-V and luminescence characteristics of a phosphorescent blue OLED (Fig. 3). Highly efficient light blue luminescence was observed with 38cd/A and CIE color index of (0.16, 0.31) at 1,000 cd/m^2.

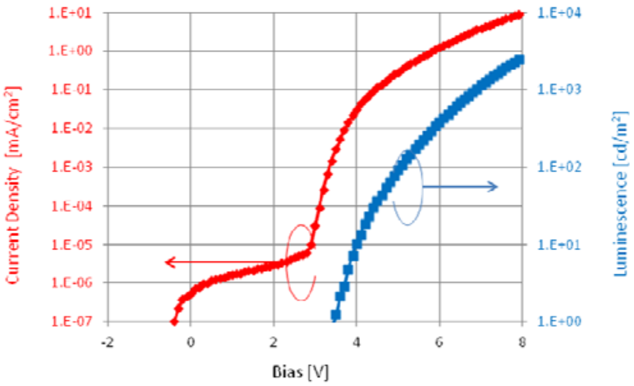

Fig.3. I-V and luminescence characteristic of phosphorescent blue OLED; Glass /ITO(150nm) /TcTa(70nm)/mCP:Firpic(6%,40nm) /TmPyPB(40nm)/Al(150nm). CIE color index and efficiency are (0.16, 0.31) and 38.0 cd/A at 1,000cd/m^2, respectively.

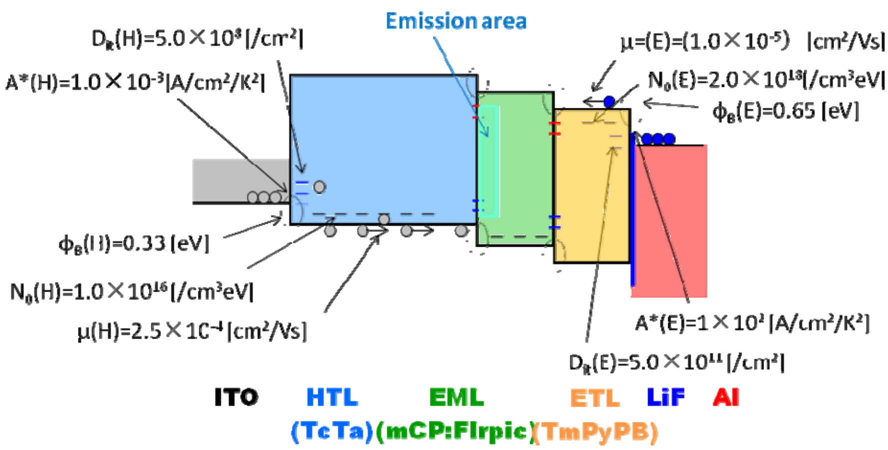

Fig.4. Estimated device parameters of hole and electron injection side are illustrated in standard phosphorescent blue OLED.

Fig. 4 shows the estimated device parameters of the hole and electron injection interfaces and emission area which was investigated using a FIrpic-doped OLED. We believe it is very important to analyse the condition at the hole injection interface of the emission layer in order to understand degradation mechanisms.

Summary

We have proposed a novel numerical model for Schottky I-V and IS measurements and determined the device parameters for a phosphorescent blue OLED.

References

[1] O. W. Richardson O W 1914 *Philos. Mag.* **28** 633
[2] Scott J C 2003 *J. Vac. Sci. Tech.* A **21** 521
[3] Okachi T, Nagase T, Kobayashi T and Naito H 2008 *Jpn. J. Appl. Phys*. **47** 8965
[4] Hirai T, Weber K, Li J H, Bown M and Ueno K 2011 *SID International Symposium* p181
[5] Hirai T, Weber K, O'Connell J, Bown M and Ueno K 2011 *SSDM International Symposium* B-1-6
[6] Tse S C, Tsang S W and So S K 2006 *J. Appl. Phys.* **100**, 063708
[7] Sze S M 1981 *Physics of Semiconductor Devices* 2nd edition (Wiley) p 257