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Determination of Traps’ Density of State in OLEDs from Current–Voltage Analysis *

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A simple method to determine the traps’ density of state (DOS) in organic light-emitting diodes (OLEDs) by manipulating the current–voltage (I–V) characteristic of the devices at room temperature is introduced. In particular, the trap-dependent space-charge limited current formula is simplified to obtain effective density of traps. In this study, poly[(9,9-di-n-octylfluorenyl)-2,7-diy]-alt-(benzo[2,1,3]thiadiazol-4,8-diyl)] (F8BT) and 2-Methoxy-5-(3',7'-dimethylctoxyloxy) benzene-1,4-diacetonitrile (OC10C10-PPV) are selected as the OLEDs emissive layer. The trap DOS of F8BT- and OC10C10-PPV-based OLEDs are calculated in the magnitudes of 10^3 m^-3 and 10^2 m^-3, respectively. In addition, the results agree with the other conventional method which is used to determine the trap DOS in OLEDs. This calculation technique may serve as a robust and reliable approach to obtain the trap DOS in OLEDs at room temperature.

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Since first reported by Tang et al.,[1] organic light-emitting diodes (OLEDs) have been intensively studied due to their potential applications in solid-state lighting and display. There are several advantages of OLEDs as a display compared with that of the recent liquid crystal display (LCD) including non-backlight function, slimmer in thickness, wide viewing angle, high brightness, faster to respond and low power consumption.[2] The OLED-based display devices can also be more cost-effective to manufacture compared with LCDs and plasma displays. Despite all the great features, a few drawbacks still yet limit their efficiency.

Optoelectronic properties of OLEDs depend largely on the distribution of localized states in the band gap of the materials.[3] There are several factors that contribute to trap states in organic semiconductors. Charge carrier traps are caused by chemical impurities formed during the material’s synthesis. The chemical impurities may cause structural defects by distorting the host lattice.[4] Chemical impurities also tend to accumulate in the regions where the structural disorder[4] is high and at the surface of a crystal.[6] A theoretical study has pointed out that large fluctuations in the transfer integral of thermal motion in the molecules can result in a tail of trap states extending from the valence-band edge into the gap, and the band tail is of temperature dependence. Some experimental evidence suggests that trap states due to thermal motion of molecules play a role in the samples with a low trap density.[7–9]

Tsaí et al.[10] reported the effect of traps in OLEDs. Not only can traps reduce the current generated from a fixed voltage, but also it strongly increases the transient time which causes slow charge carrier transportation in the devices. Traps also alter the recombination region close to the cathode and thus reduce the external quantum efficiency and device performance. Therefore, studies of trap dependences in charge transport become important to provide a foundation to understand the electroluminescence (EL) mechanism in devices.

Kumar et al.[11] proposed a technique to estimate trap density from temperature dependence of an I–V characteristic. On the other hand, in the method of Lang et al.[12] the free charge carriers are ignored when estimating the trap density. Horowitz et al.[13] obtained that the trap DOS has to be calculated for each different temperature. The trap DOS from the measurement needs to be repeated for different temperatures until the value from the calculation with different measurements coincides with each other after adjusting μ0Nc, where μ0 is defined as a microscopic mobility, and Nc is the effective density of states in the conduction band.

This work is mainly focused on introducing a simple calculation method to determine trap DOS in OLED by manipulating the I–V characteristic of the device at room temperature. F8BT and OC10C10-PPV have been chosen as emissive materials for OLEDs. The obtained results were compared with other methods. The advantage of the proposed technique is that the trap DOS is monitored in a device under operational conditions. In application stage, OLEDs are normally operated at room temperature, thus it is significant to study the trap’s DOS under this condition. This technique is also simple and direct, which is just using an extended analysis of the I–V characteristic of the device.

Poly(9,9-diocytfluorene-alt-benzothiadiazole) (F8BT)[14] and (2-Methoxy-5-(3',7'-dimethylctoxyloxy) -benzene-1,4-diacetonitrile) (OC10C10-PPV)[15] emissive polymer were selected in this study due to their excellent emission properties. These materials are also known as electron acceptors in organic solar cells. The chemical structures of these polymers are shown in Fig. 1. The HOMO and LUMO for F8BT are 5.1 and 3.1 eV, respectively. For the OC10C10-PPV, the

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values are 5.0 and 2.8 eV, respectively. The energy gaps for F8BT and OC1C10-PPV are 2.0 and 2.2 eV, respectively.

\[
\begin{align*}
\text{(a)} & \quad \text{Au}(50 \text{ nm}) \\
\text{PEDOT:PSS}(70 \text{ nm}) & \\
\text{(b)} & \quad \text{Al}(50 \text{ nm}) \\
\text{ZnO}(70 \text{ nm}) & \\
\text{ITO}(10 \text{ nm}) & \\
\text{F8BT}(870 \text{ nm}) & \\
\text{Ca}(10 \text{ nm}) & \\
\text{MoO}_3 (10 \text{ nm}) & \\
\text{F8BT}(870 \text{ nm}) & \\
\text{ITO}(10 \text{ nm}) & \\
\text{Glass}(50 \text{ nm}) & \\
\end{align*}
\]

**Fig. 1.** Chemical structures of (a) F8BT and (b) OC1C10-PPV.

To reduce the complexity of the charge transport mechanism and its kinetic, single carrier devices are selected, which are the hole-only device (HOD)\(^{[16]}\) and the electron-only device (EOD).\(^{[17]}\) For F8BT, the HOD and EOD were constructed as ITO/PEDOT:PSS/F8BT/MoO3/Au and ITO/ZnO/F8BT/Ca/Al, respectively, as shown in Fig. 2. The energy band diagram of F8BT-HOD is shown in Fig. 3(a). The role of the MoO3 layer is to prevent electron injection from Au into F8BT layer. In the F8BT-EOD device, the energy band diagram is shown in Fig. 3(b). The ZnO layer acts as a hole blocking layer to avoid hole injection from ITO, while Ca metal will facilitate electron injection from Al due to its low work function.

For OC1C10-PPV, the single carrier devices were constructed as ITO/OC1C10-PPV/Au (Fig. 4(a)) for HOD, and ITO/Al/OC1C10-PPV/Ba/Al (Fig. 4(b)) for EOD. In the HOD, the work functions of ITO and Au are close to the HOMO level of OC1C10-PPV, thus making electron injection become difficult since the energy gap between the Au electrode and LUMO level is very large. Al in OC1C10-PPV EOD serves as a hole blocking layer between ITO anode and the OC1C10-PPV, since Al work function creates a large energy gap with its HOMO level. Al cathode and the LUMO level have a huge energy gap. Thus Ba metal acts as an electron injection layer due to the fact that its low work function is close to the LUMO level.

Charged carrier transportation in OLEDs can be understood by the \(I-V\) measurement. Transportation phenomena in the steady-state conduction occur when neither the number of charge carrier nor the local electric field changes with time. The current is given by

\[
J = qn\mu E,
\]

where \(n\) refers to the charge carrier concentration, \(q\) is the Coulomb electric charge, \(\mu\) is the mobility of the charge, and \(E\) is the electric field. In an ideal ohmic electrode contact, there is no potential barrier for injection, thus the ohmic electrodes are capable of providing an infinite supply of charge carriers. It is possible to derive the trap-free dielectric, so-called Child’s law by making use of Poisson’s equation\(^{[18]}\)

\[
J = \frac{9}{8} \varepsilon V^2 d^3,
\]

where \(\varepsilon\) is the dielectric constant, \(V\) is the applied voltage, and \(d\) is the sample thickness. The origin of deviation from Ohm’s law is that the solid is unable to transport all the injected charge. Accumulation of charges may occur, limiting the conducting current. This effect is known as the space charge limited current (SCLC). If traps exist in the solid, the SCLC would decrease by several orders of magnitude.\(^{[19]}\) Rose et al. argues that neither the field distribution nor the charge density should be altered by trapping.\(^{[20]}\) Thus the relationship between current and voltage needs to be modified by introducing a trap limiting parameter \(\theta\), which establishes the proportion of trapped charge to the free charge.

\[
\begin{align*}
\text{(a)} & \quad \text{MoO}_3 \\
\text{F8BT}(10 \text{ nm}) & \\
\text{ITO}(870 \text{ nm}) & \\
\text{Ca}(10 \text{ nm}) & \\
\text{MoO}_3 (10 \text{ nm}) & \\
\text{F8BT}(870 \text{ nm}) & \\
\text{ITO}(10 \text{ nm}) & \\
\text{Glass}(50 \text{ nm}) & \\
\end{align*}
\]

**Fig. 2.** Single layer devices of (a) hole-only and (b) electron-only used in this work.

\[
\begin{align*}
\text{(a)} & \quad \text{3.3} \\
\text{7.4} & \\
\text{HOMO} & \\
\text{LUMO} & \\
\text{MoO}_3 & \\
\text{F8BT} & \\
\text{Au} & \\
\text{Ba} & \\
\end{align*}
\]

**Fig. 3.** F8BT device energy band diagrams of (a) HOD and (b) EOD.

\[
\begin{align*}
\text{(a)} & \quad \text{3.3} \\
\text{7.4} & \\
\text{HOMO} & \\
\text{LUMO} & \\
\text{MoO}_3 & \\
\text{F8BT} & \\
\text{Au} & \\
\text{Ba} & \\
\end{align*}
\]

**Fig. 4.** OC1C10-PPV device energy band diagrams of (a) HOD and (b) EOD.

The current density is

\[
J = \frac{9}{8} \theta Q^{2} d^3,
\]

where \(n_t\) is the density of trapped charges, and \(n\) is the density of mobile carriers. In a real case, traps are more likely to be distributed in energy rather than exist at discrete levels.\(^{[21]}\) The injected carriers are expected to be trapped shifting the quasi-Fermi level upwards. Looking at an exponential density of traps, and under the approximation that all the trapping states are filled below the Fermi level, the current–potential characteristic can be written as\(^{[22]}\)

\[
J = q\mu n_c \left( \frac{\varepsilon}{q H_t} \right)^{\ell} (\ell + 1)^{\ell + 1} V^{\ell + 1} d^{2\ell + 1},
\]

\[
\ell = \frac{T_c}{T},
\]
where \( q \) refers to the Coulomb electric charge, \( \mu \) is the mobility of the charge carrier, \( \varepsilon \) is the dielectric constant, \( N_c \) is the effective density of states in the transport level, \( H_t \) is the effective density of traps, \( T_c \) is the characteristic trap temperature, \( T \) is the operating temperature, and \( d \) is the thickness of the sample. In the work presented by Kumar et al.,[1] Eq. (5) can be simplified and solved. Further details and discussion are not given in this study since they have already been carried out by Kumar et al.

From the solution provided, Eq. (5) is rearranged to estimate the values of \( H_t \), which shows that \( H_t \) depends on the voltage and current density. Thus \( H_t \) can be calculated from the \( J-V \) characteristic of the devices.

MATLAB (matrix laboratory) is a numerical computing environment software and fourth-generation programming language developed by MathWorks. MATLAB is used to calculate and plot the value of trap density. In this work, we consider two similar cases while with a different type of organic material as the emissive material.

For the first case, an HOD and an EOD consist of F8BT materials as shown in Fig. 2. Its energy band diagram is shown in Fig. 3. The fabrication methods of HOD and EOD have already been explained in Ref. [23] and thus not presented in this study since the focus in this work is to evaluate trap density. The \( J-V \) plots of the HOD and EOD are shown in Fig. 5. Here the data are extracted from the original manuscript. Device parameters for F8BT-type of materials are listed in Table 1, which is used to estimate \( H_t \), trap density of respective devices. The plot of the simulated trap density with respect to the voltage of the device is shown in Fig. 6.

**Table 1.** The parameters used for the estimation of trap density for the F8BT-type material.

<table>
<thead>
<tr>
<th></th>
<th>Electron only device</th>
<th>Hole only device</th>
</tr>
</thead>
<tbody>
<tr>
<td>( N_c ), density of state in transport level (m(^{-3}))</td>
<td>2.5 \times 10^{26}</td>
<td>2.5 \times 10^{26}</td>
</tr>
<tr>
<td>( \mu ), mobility of carrier (m(^2)V(^{-1})s(^{-1}))</td>
<td>2 \times 10^{-8}</td>
<td>3 \times 10^{-10}</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>( q ), electric charges (C)</td>
<td>1.6 \times 10^{-19}</td>
<td>1.6 \times 10^{-19}</td>
</tr>
<tr>
<td>( d ), thickness of sample (m)</td>
<td>8.7 \times 10^{-7}</td>
<td>8.7 \times 10^{-7}</td>
</tr>
<tr>
<td>( k ), Boltzmann’s constant (eV-K(^{-1}))</td>
<td>8.62 \times 10^{-5}</td>
<td>8.62 \times 10^{-5}</td>
</tr>
<tr>
<td>( T_c ), characteristic trap temperature (K)</td>
<td>1500</td>
<td>1500</td>
</tr>
<tr>
<td>( \varepsilon_s ), permittivity of sample</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>( \varepsilon_0 ), permittivity of air</td>
<td>8.85 \times 10^{-12}</td>
<td>8.85 \times 10^{-12}</td>
</tr>
</tbody>
</table>

**Table 2.** The parameters used for the estimation of trap density for the OC\(_1\)C\(_{10}\)-PPV-type material.

<table>
<thead>
<tr>
<th></th>
<th>Electron only device</th>
<th>Hole only device</th>
</tr>
</thead>
<tbody>
<tr>
<td>( N_c ), density of state in transport level (m(^{-3}))</td>
<td>2.5 \times 10^{25}</td>
<td>2.5 \times 10^{24}</td>
</tr>
<tr>
<td>( \mu ), mobility of carrier (m(^2)V(^{-1})s(^{-1}))</td>
<td>2 \times 10^{-9}</td>
<td>5 \times 10^{-11}</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>295</td>
<td>295</td>
</tr>
<tr>
<td>( q ), electric charges (C)</td>
<td>1.6 \times 10^{-19}</td>
<td>1.6 \times 10^{-19}</td>
</tr>
<tr>
<td>( d ), thickness of sample (m)</td>
<td>7.4 \times 10^{-7}</td>
<td>9.8 \times 10^{-8}</td>
</tr>
<tr>
<td>( k ), Boltzmann’s constant (eV-K(^{-1}))</td>
<td>8.62 \times 10^{-5}</td>
<td>8.62 \times 10^{-5}</td>
</tr>
<tr>
<td>( T_c ), characteristic trap temperature (K)</td>
<td>1500</td>
<td>1500</td>
</tr>
<tr>
<td>( \varepsilon_s ), permittivity of sample</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>( \varepsilon_0 ), permittivity of air</td>
<td>8.85 \times 10^{-12}</td>
<td>8.85 \times 10^{-12}</td>
</tr>
</tbody>
</table>

For the second case, a similar single carrier device is considered. The organic material F8BT is replaced with OC\(_1\)C\(_{10}\)-PPV. The \( I-V \) plots for the HOD and EOD of the device are shown in Fig. 7. The corresponding parameters used to estimate the trap densities are listed in Table 2. Figure 8 shows the...
corresponding value of trap density simulated for the OC$_1$C$_{10}$-PPV type material.

![Graph](image_url)

**Fig. 7.** Current $J$ versus voltage $V$ for the OC$_1$C$_{10}$-PPV material consisting of HOD and EOD.\cite{25}

![Graph](image_url)

**Fig. 8.** Trap density $H_t$ versus voltage $V$ for HOD and EOD of the OC$_1$C$_{10}$-PPV-type material.

From Fig. 6, we can observe that for the first case, HOD has a higher depth of the trap density compared with the EOD. In comparison of the device parameter data in Table 1, it is found that the mobility carrier is the main factor contributing to the depth of trap density. The lower the mobility of the device is, the higher the depths of trap density are expected, which is in agreement with the findings reported by Horowitz et al.\cite{23} Horowitz presented that $H_t$ may be divided into deep states and tail states. Deep state densities could originate from dangling bonds or from grain boundaries. A scanning electron micrography (SEM) result should be able to yield the grain size of the material which is proportional to the density of deep states. Moreover, a backward transition from hopping to trapping can also be induced in the accumulation layer by increasing the voltage bias. As the voltage increases, more trap levels are filled with injected charges. Eventually, all deep traps will be filled, and the dominant transport mechanism will switch back to multiple trapping. Evidence for such transition is the very fast increase of the saturation current with the voltage bias.

In Fig. 9, the plots of trap density are compared with the experimental results of the trap density value of F8BT materials as reported in Ref. \cite{24}. The experimental results are temperature dependent. Since the goal of our work, here we present a method to estimate trap density at room temperature; evidently we manage to achieve this just as shown in the figure. From Fig. 10, we observe the similar trend for case 2 in which the trap density of HOD is much higher than the EOD. However, the magnitudes of trap density of case 2 are slightly lower than those of case 1. The results are compared with those reported by Mandoc,\cite{22} as shown in Fig. 10. The results are found to be comparable with each other. Nicolai et al.\cite{22} have also reported that the number of electron-traps amounts to $3\times10^{23}$ traps/m$^2$ is centered at an energy of 3.6 eV below the vacuum level, with a typical distribution width of 0.1 eV, which is quite close to the results obtained for case 2.

![Graph](image_url)

**Fig. 9.** Comparison of the total trap density for F8BT materials between this method and that reported by others.\cite{24}

![Graph](image_url)

**Fig. 10.** Comparison of the total trap density for OC$_1$C$_{10}$-PPV materials between this method and that reported by others.\cite{22}

In summary, the HOD has a higher trap density than the EOD due to its main contribution in nature of the device itself, and the HOD has a lower mobility than the EOD. Other factors such as molecular bonding and grain-size are not discussed thoroughly since more information, such as SEM or x-ray diffraction results, is needed. We manage to estimate the trap density, and the results are quite comparable with those reported by others. It is proven that this method can be used to estimate trap density for single carrier devices at room temperature.
References

[27] Chua L L et al 2005 Nature 434 194