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Comparison Between Mobility Models in Organic Semiconductors

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Over the years, a large number of fundamentally different models have been proposed to describe the charge transport in organic semiconductor materials. The models available in literature can be divided into two classes: (i) band-like models, assuming the transport in extended delocalized states; (ii) gap-states transport models if the charge carriers move from one localized site to another by thermal-assisted tunneling. Usually the first class is more suitable for polycrystalline or high-mobility semiconductors whereas the second class is usually used for amorphous materials. In many mobility models, an essential ingredient is the Density of States (DOS) which describes the trap distribution in the gap of an organic semiconductor. Usually it is assumed to be a Gaussian function for OLED [1] and an exponential function for OTFT [2].

In this work we study three mobility models, which are usually used to describe the charge transport and/or to calculate the drain current of OTFTs:

1. Multiple Trapping and Release (MTR) [3]
2. Variable Range Hopping (VRH) [4]

These are relevant models widely used in literature, and they have a completely different physical background among them. The MTR is a band-like model and it was originally introduced by Shur and Hack [6] for amorphous silicon TFTs and later used by Horowitz [3] for OTFTs. The VRH was proposed by Vissenberg and Matters [4] for the modelling of the field-mobility in OTFTs. It considers the hopping percolation of charge carriers between localized states. The MNR is an empirical relation proposed by Meyer and Neldel [5]. It states that in a thermally activated process an increase in the activation energy $E_A$ is partially compensated by an increase in the prefactor. Few efforts have been made to compare all these models [7].

In this work, we used these models in order to fit the field-effect mobility of several organic semiconductors used as active layers in OTFTs. Our goal is to understand if it is possible to discriminate the transport model from the measured field-effect mobility, investigating the physical relationships among them. By means of the definition of a function $\vartheta$, we also give some guide lines for the choice of the appropriate model and its range of application.

Since we investigate the mobility in OTFTs, we consider a single exponential DOS as approximation of the actual one in the range of interest. We consider the following analytical models:

\[
\mu_{\text{MTR}} = \frac{\sigma_0}{q} \left[ \frac{T}{T_c} \sin \left( \frac{\pi T}{T_c} \right) \right]^{\frac{1}{\alpha}} \frac{V}{C} \quad \mu_{\text{VRH}} = \frac{\sigma_0}{q} \left[ \frac{T}{T_0} \sin \left( \frac{\pi T}{T_0} \right) \right]^{\frac{1}{\gamma}} \quad \mu_{\text{MNR}} = \mu_0 \exp \left( \frac{E_A}{E_{\text{MN}}} \right) \exp \left[ -\frac{E_A}{k_B T_{\text{MN}}} \right]
\]

\[\sigma_0 \quad \alpha \quad T_0 \quad T_c \quad N_t = 1/a^3 \quad \mu_0 \quad E_{\text{MN}} \quad k_B \quad T_{\text{MN}} \quad E_a(V_{GATE})\]

$\sigma_0$ and $\mu_0$ are the conductivity and the mobility prefactors respectively, $\sigma_0$ is the band-conductivity, $N_t$ the total number of traps in the gap, $\alpha$ is the average interstate distance, $1/\alpha$ is the wavefunctions overlap parameter and it is related to the stacking properties of the molecules. $T_0$, $T_c$ and $T_{\text{MN}}$ are the characteristic temperatures, which take into account the energetic disorder of the material (proportional to the DOS width for the MTR and VRH). Since we used the same DOS parameters for the models shown above, it results: $T_c = T_0 = T_{\text{MN}}$ and with the hypothesis of an exponential DOS it is possible to demonstrate [8] that $T_{\text{MN}} = T_c$.

In order to directly compare the MTR and VRH models, we introduce the function $\vartheta(\lambda, \gamma, \chi)$ which gives: $\mu_{\text{VRH}} = \vartheta \mu_{\text{MTR}}$, where $\chi = a/\alpha^2$ is an index of the charge carriers localization in the traps, $\lambda = \sigma_0/\alpha_0$ and $\gamma = T_c / T$ being $T_c$ the characteristic temperature. The quantity $\vartheta$ as a function of temperature $T$ allows to distinguish between the two mobility models. On the other hand, we observe that MTR and VRH models have the same carrier concentration $c$ dependency ($T_c = T_0$). Hence, despite the results in [7], carrier density dependency of $\mu$ does not discriminate the transport mechanism.

The three mobility models have been compared in Figs 1-6 with experimental field-effect mobility collected from literature for different materials (both small-molecules and polymers). The extracted model parameters are reported in Tab. 1, and all values are in a physically acceptable range. All the semiconductors show Arrhenius temperature dependence and hence, the experimental data can be easily fitted with MNR model (solid curves with circles) with activation energy $E_a$ dependent on the gate-voltage. We observe that the characteristic temperature $T_c$ reflects the level of energetic disorder in the material. In fact, evaporate-processed Pentacene (Pentacene\_1, Pentacene\_2) has lower $T_c$ than the solution-processed one (Pentacene\_3), because during evaporation the molecules reach better stacking properties.

We found that MTR model (blue solid lines in Figs. 1-6) is also suitable for the description of organic semiconductors in a wide range of temperatures and charge concentrations, because it accurately fits the measured mobility of all the materials.
The VRH model (red dashed lines) works well in a limited range of temperatures. At low temperatures $T$ (Fig. 1), the VRH model gives a mobility almost independent of $T$ and we see that at a certain low temperature $T^*$ the predicted mobility starts to increase by decreasing $T$. This behavior is not physically consistent with the model hypothesis. We also found that $T^*$ depends on the parameter $1/\alpha$; i.e. if $1/\alpha$ increases then $T^*$ increases too, enhancing the above mentioned behavior.

The insets of Figs. 1 and 2 show the function $\theta$ in the temperature range of the experimental data. In the case of NRS-PPV, MTR and VRH cannot be distinguished because both models fit the experimental data, and the function $\theta$ is close to 1. On the other hand, in Pentacene_3 function $\theta$ tends to 1 only in a small range of temperatures and it diverges at low temperatures. Therefore, MTR and VRH models differ. In fact, only MTR fits the experimental data in the whole range of temperatures.

The results suggest two more things: first, a wide range of temperature data is necessary to discriminate the transport mechanism, and second, VRH seems to over-estimate $\mu$ at low temperatures. We remark the proposed function $\theta$, which gives a mapping between MTR and VRH models. Moreover, we found that if $1/\alpha$ is smaller, a better mapping between MTR and VRH is achieved and the two models cannot be distinguished.

**Fig. 1-6 legend:** Diamonds experimental data at different $V_{\text{GATE}}$, blu solid lines MTR, red dashed lines VRH, solid line with circles MNR

<table>
<thead>
<tr>
<th>Ref.</th>
<th>$T_c$ [K]</th>
<th>$\alpha_0$ [S/m]</th>
<th>$N_{\text{fit}}=1/\alpha^*\ [1/cm^2]$</th>
<th>$\alpha_0 [S/m]$</th>
<th>$1/\alpha [\text{Å}]$</th>
<th>$\mu_0 [\text{cm}^2/\text{Vs}]$</th>
<th>$\epsilon_{\text{G1}}V_{\text{G1}}$</th>
<th>$\epsilon_{\text{G2}}V_{\text{G2}}$</th>
<th>$\epsilon_{\text{G3}}V_{\text{G3}}$</th>
<th>$\chi=a/\alpha^*[-]$</th>
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<td>Pentacene_1</td>
<td>[9]</td>
<td>375</td>
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<td>0.75 $10^{21}$</td>
<td>3.50 $10^{-7}$</td>
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<td>Pentacene_2</td>
<td>[4]</td>
<td>385</td>
<td>4.8 $10^7$</td>
<td>4 $10^{21}$</td>
<td>1.60 $10^{-7}$</td>
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<td>Pentacene_3</td>
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<td>5.76 $10^7$</td>
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<td>6 $10^{-7}$</td>
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<td>P3HT</td>
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<td>3</td>
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<td>OC$<em>{2}$C$</em>{10}$-PPV</td>
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<td>540</td>
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**References:**