Effect of the electric field and effective temperature on the mobility in disordered organic semiconductors

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The theoretical description of the effect of the electric field and effective temperature on the mobility is yet a matter of controversy related to the charge transport in disordered organic semiconductors. In this paper, a systematic study of the hole transport in blue-emitting polymers as poly(9,9-dioctylfluorene) (PFO) has been performed. From an analysis of the layer thickness and temperature dependent current density-voltage characteristics of the PFO hole-only devices, it is found that consistent descriptions with equal quality are obtained by using the extended Gaussian disorder model (EGDM), extended correlated disorder model (ECDM), and effective temperature extended Gaussian disorder model (ET-EGDM). The extracted values of the width of the Gaussian density of states σ from the three models are rather similar and observed to fall in the range of typical values. However, the extracted values of average intersite distance a from the three models are quite different. The value of a from the ET-EGDM is very close to the typical values, and is obviously smaller than that from the EGDM and is obviously higher than that from the ECDM, indicating that the ET-EGDM provides a more appropriate description of the electric field dependence of the mobility than the EGDM and ECDM.

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1. Introduction

Disordered organic semiconductors are currently investigated due to their easy manufacturing and possible applications in optoelectronic devices, such as organic light emitting diodes (OLEDs), organic photovoltaic cells (OPV), and organic field effect transistors (OFETs) [1-8]. Before full-scale commercialization of these organic devices is possible, several important challenges must be overcome. This includes enhancement of the charge carrier transport and environmental stability of disordered organic semiconductors. Thus, an understanding of the charge transport properties is very important to design and synthesize better materials that can further improve the performance of organic devices [9-11].

For disordered organic semiconductors, charge carrier transport is commonly understood to occur via incoherent thermally activated hopping of charge carriers between randomly distributed localized states. The most important parameter characterizing the charge transport properties is the charge carrier mobility μ. In the past two decades, various methods have been proposed to calculate the mobility function [12-22]. The pioneering work of Bässler et al. used kinetic Monte Carlo simulation, and the random energy is described by Gaussian Density of States (DOS), leading to the Gaussian disorder model (GDM) [12], within which spatial correlations between the transport site energies are absent. Alternatively, it was suggested that the presence of dipole moments can give rise to spatial correlation between the site energies [13, 14], leading to the correlated disorder model (CDM). Later, it was realized that, apart from the dependence of the mobility μ on the electric field E and temperature T, there is a strong dependence on the carrier density p [15, 16], giving rise to the extended versions of the GDM and CDM, the EGDM and ECDM [17, 18], respectively. For small but realistic electric fields, the field dependence of the mobility is within the ECDM much stronger than within the EGDM. On the other hand, the charge carrier density dependence is for the ECDM slightly weaker than the EGDM. The EGDM and ECDM are sometimes considered universal, and are the basis for commercially available organic devices simulation software [19, 20]. However, the methodology to derive the EGDM and ECDM has been heavily criticized for giving an inappropriate description of especially the field dependence of the mobility [23-25]. To better describe the charge transport properties, we proposed an effective temperature extended Gaussian disorder model (ET-EGDM) by inserting the field dependent effective temperature instead of the real temperature into the EGDM [26]. It is shown that the ET-EGDM provides much stronger electric field dependence of the mobility than the EGDM, the effective temperature responsible for the combined effects of the electric field and real temperature on the mobility.

The question now arises whether the ET-EGDM can

provide a better description for the charge transport in disordered organic semiconductors than the EGDM and ECDM, and whether it will be possible to give an appropriate field dependence of the mobility. In this paper, we will investigate whether such an extensive analysis can be given for the charge transport in blue-emitting polymers as poly(9,9-dioctylfluorene) (PFO). From an analysis of the layer thickness and temperature dependence of the current density-voltage ($J-V$) characteristics of the PFO hole-only device, it is found that consistent descriptions with equal quality can be obtained within the EGDM, ECDM, and ET-EGDM. However, a more realistic value of average intersite distance is obtained within the ET-EGDM than within the EGDM and ECDM. This is an indication that the ET-EGDM can provide a more appropriate description of the electric field dependence of the mobility than the EGDM and ECDM.

2. Models and methods

A commonly employed mobility model has been developed by Pasveer et al. on basis of numerical transport simulations accounting for hopping on a simple cubic lattice with uncorrelated Gaussian disorder [17]. For historical reasons this model is often referred to as the EGDM. In the EGDM the mobility can be expressed as

$$\mu(T,p,E)\approx\mu_0(T)f(T,E)\exp[\frac{1}{2}\left(\hat{\sigma}^2-\hat{\sigma}\right)\left(2pa^3\right)^{\delta}] \quad (1)$$

$$\mu_0(T)=\mu_0 b_1\exp(-b_2\hat{\sigma}^2) \quad (2)$$

$$f(T,E)=\exp\left\{0.44\left(\hat{\sigma}^{3/2}-2.2\right)\left[\sqrt{1+0.8\left(\frac{eaE}{\sigma}\right)^2}-1\right]\right\} \quad (3)$$

$$\delta\equiv 2\frac{\ln(\hat{\sigma}^2-\hat{\sigma})-\ln(\ln 4)}{\hat{\sigma}^2},\quad \mu_0\equiv\frac{a^2\nu_0 e}{\sigma} \quad (4)$$

where $\mu_0(T)$ is the mobility in the limit of zero carrier density and electric field, $f(T,E)$ is the field dependent factor, μ_0 is the mobility prefactor, $b_1=1.8\times10^{-9}$, $b_2=0.42$, $\hat{\sigma}\equiv\sigma/k_BT$ is the reduced disorder, σ is the width of Gaussian density of states (DOS), e is the charge of the carriers, a is the lattice constant (average intersite distance) and ν_0 is the attempt-to-hop frequency.

In addition to uncorrelated energetic disorder, the presence of molecular dipoles may give rise to spatial correlations in the energy distribution of the sites. Bouhassoune et al. employed the same methodology as in the EGDM, but for an energy landscape with Gaussian disorder that result from randomly oriented dipole moments of equal magnitude on all lattice sites, leading to the extended correlated disorder model (ECDM) [18]. The mobility can be described as follows:

$$\mu(T,p,E)=[(\mu_{low}(T,p,E))^{q(\hat{\sigma})}+(\mu_{high}(p,E))^{q(\hat{\sigma})}]^{1/q(\hat{\sigma})} \quad (5)$$

$$q(\hat{\sigma})=2.4/(1-\hat{\sigma}) \quad (6)$$

with $\mu_{low}(T,p,E)$ is the mobility in the low-field limit, and $\mu_{high}(p,E)$ is the mobility in the high-field limit.

$$\mu_{low}(T,p,E)=\mu_0(T)g(T,p)f(T,E,p) \quad (7)$$

$$\mu_0(T)=1.0\times10^{-9}\mu_0\exp(-0.29\hat{\sigma}^2) \quad (8)$$

where $g(T,p)$ and $f(T,E,p)$ are the dimensionless mobility enhancement functions.

$$\mu_{high}(p,E)=\frac{2.06\times10^{-9}}{E_{red}}\mu_0(1-pa^3) \quad (9)$$

where E_{red} is the average reduced field.

The EGDM and ECDM are sometimes considered universal and they are the basis for commercially available organic devices simulation software [19, 20]. However, the methodology followed to derive the EGDM and ECDM parametrizations has been heavily criticized for giving an inadequate description of especially the field dependence of the mobility [23-25].

A milestone for the theoretical description of the dependence $\mu(E)$ in materials with hopping transport was set by Shklovskii for the case $T=0$, who recognized that the effect of the electric field on the carrier mobility is determined by the product $eE\alpha$ (α is the localization length) [27]. For the case $T\neq0$, Shklovskii and successors argued that the combined effects of the electric field and temperature on the mobility can be expressed in the form of an effective temperature [28, 29]:

$$T_{eff}=\left[T^2+(\gamma\frac{eE\alpha}{k_B})^2\right]^{1/2} \quad (10)$$

with $\gamma\approx0.67$. The validity of the approach based on the effective temperature has been confirmed in numerous studies [23-25].

In principle, Eq. (10) can be combined with any model that describes the temperature dependent mobility of a hopping system by replacing the temperature T by the effective temperature T_{eff}. To describe the combined effects of electric field and temperature on the mobility,

we will improve the EGDM expression by inserting the field dependent effective temperature T_{eff}, instead of the real temperature T, into the temperature dependence of the mobility:

$$\mu(T, p, E) = \mu(T_{eff}, p) f(T_{eff}, E) \tag{11}$$

where

$$\mu(T_{eff}, p) = \mu_0(T_{eff}) \exp\left[\frac{1}{2}(\hat{\sigma}^2 - \hat{\sigma})(2pa^3)^{\delta}\right] \tag{12}$$

$$f(T_{eff}, E) = \exp\left\{0.44\left(\hat{\sigma}^{3/2} - 2.2\right)\left[\sqrt{1 + 0.8\left(\frac{eaE}{\sigma}\right)^2} - 1\right]\right\} \tag{13}$$

$$\mu_0(T_{eff}) = \mu_0 b_1 \exp\left(-b_2 \hat{\sigma}^2\right) \tag{14}$$

In the following, the mobility model Eqs.(10)-(14) will be referred to as the effective temperature extended Gaussian disorder model (ET-EGDM).

3. Results and discussion

In this section, we will apply the EGDM, ECDM, and our improved model (ET-EGDM) as described in section 2 to the PFO hole-only devices, and then compare the dependence of mobility on the electric field and carrier density from the three models. PFO is an attractive material to function as the blue host material in white OLEDs due to its efficient blue emission and high mobility. The highest occupied molecular orbital (HOMO) level of PFO is located at 5.8 eV below vacuum, leading to a significant hole injection barrier of 0.6 eV when combined with PEDOT:PSS with a work function of approximately 5.2 eV [30]. Such an injection barrier will strongly hamper the hole current and limit the device performance. Fortunately, Nicolai et al. has demonstrated that molybdenum trioxide (MoO_3) as hole injection layer can form an Ohmic contact on PFO, enabling the observation of a space-charge limited (SCL) current [31]. Apparently, the occurrence of a SCL current makes it possible to further investigate the electric field and carrier density dependence of the mobility for PFO.

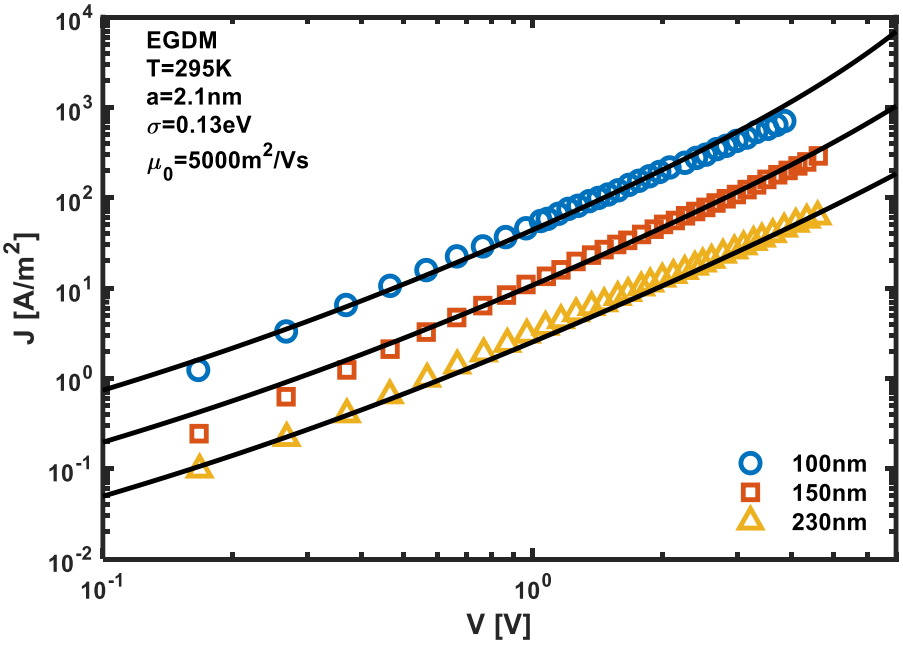

Fig. 1. Thickness dependent J-V characteristics of PFO hole-only devices. Symbols are experimental data from Ref. [31]. Lines are the numerically calculated results from the EGDM (colour online)

To explore the charge transport properties in more detail and evaluate the dependence of mobility on the electric field and carrier density, we investigate the layer thickness and temperature dependent space-charge limited current for the PFO hole-only devices. As previously described, the mobility in organic semiconductors exhibiting hopping transport depends on the temperature, electric field, and carrier density. For a system with Gaussian disorder, the mobility can be described by the EGDM, ECDM, and our ET-EGDM, in which only uses three input parameters: the width of the Gaussian density of states σ, average intersite distance a, and a mobility prefactor μ_0. The σ mainly controls its temperature and carrier density dependence, a predominantly affects its field dependence, and the mobility prefactor μ_0 determines the magnitude of the mobility. Fig. 1 shows the thickness dependent $J-V$ characteristics of hole-only devices with PFO layer

thickness of 100 nm, 150 nm, and 230 nm at room temperature. Apparently, the experimental data can be well described by using the EGDM, within which an optimal fit can be obtained using a single parameter set of a =2.1 nm, σ =0.13 eV, and μ_0 =5000 m^2/Vs. Fig. 2 depicts the temperature dependent $J-V$ characteristics of a PFO hole-only device with a layer thickness of 230 nm. It is obviously that the temperature dependent hole current could also be accurately described within the EGDM using the same parameters as the thickness dependent $J(V)$ curves. For the model parameters, the value of the disorder parameter σ is equal to the value used by Nicolai et al. [31], which is observed to fall in the range 0.06-0.16 eV (typical values of σ for organic semiconductors). The value of average intersite distance a found from the EGDM is significantly higher than the typical value of organic semiconductors (1 nm).

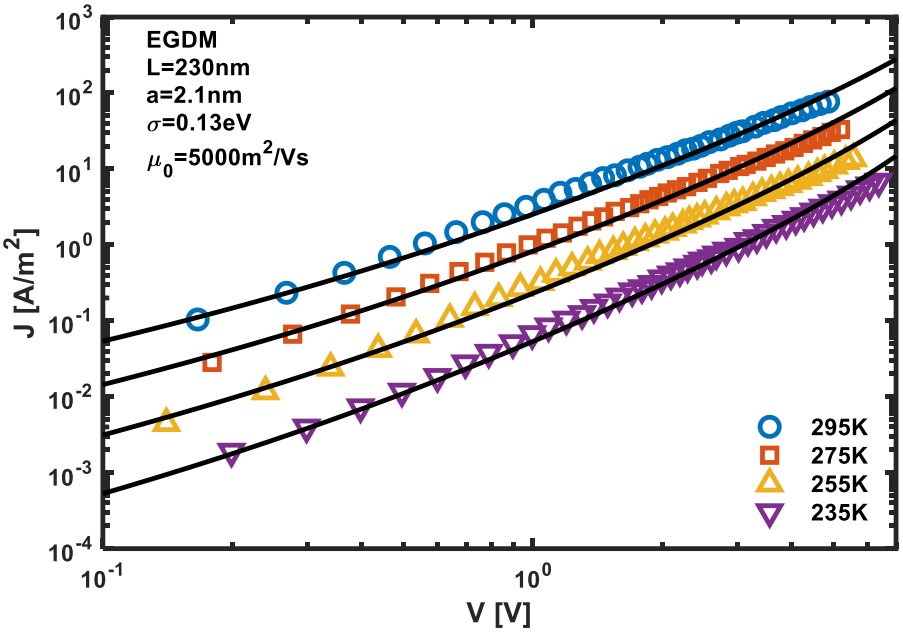

Fig. 2. Temperature dependent J-V characteristics of PFO hole-only device. Symbols are experimental data from Ref. [31]. Lines are the numerically calculated results from the EGDM (colour online)

As a next step, we consider the question whether the ECDM can also describe the $J-V$ characteristics of the PFO hole-only devices with various layer thicknesses and temperatures as good as the EGDM. When employing the ECDM, we address the question whether site-energy correlations with this specific correlation function are present in PFO. Here, we re-analyse these experimental data for the PFO hole-only devices by using the ECDM. Fig.3 and Fig.4 show the thickness and temperature dependent $J-V$ characteristics of the PFO hole-only devices, respectively. Obviously, the thickness and temperature dependent $J-V$ characteristics of the PFO hole-only devices can also be well described within the ECDM only using a single set of parameters, a =0.16 nm, σ =0.145 eV, and μ_0 =5500 m^2/Vs. It is found that the ECDM can also provide a good description for the hole transport in PFO, provided that a much smaller average intersite distance is assumed within the ECDM (0.16 nm) than the typical value (1 nm). The value of a found from the ECDM may be considered as unrealistically small (significantly lower than the typical value of organic semiconductors). This indicates that there is no correlation between the transport site energies in PFO.

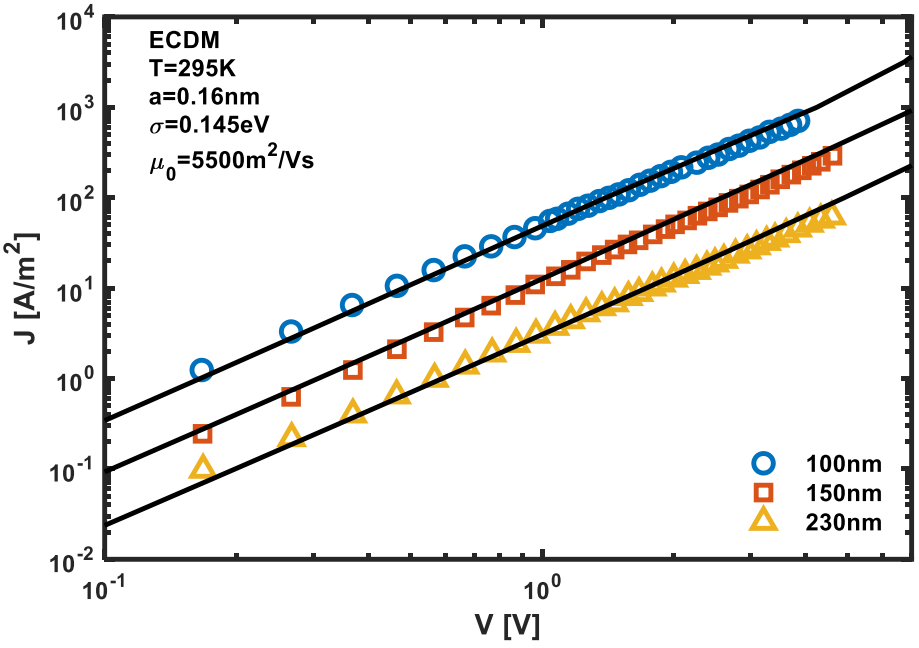

Fig. 3. Thickness dependent J-V characteristics of PFO hole-only devices. Symbols are experimental data from Ref. [31]. Lines are the numerically calculated results from the ECDM (colour online)

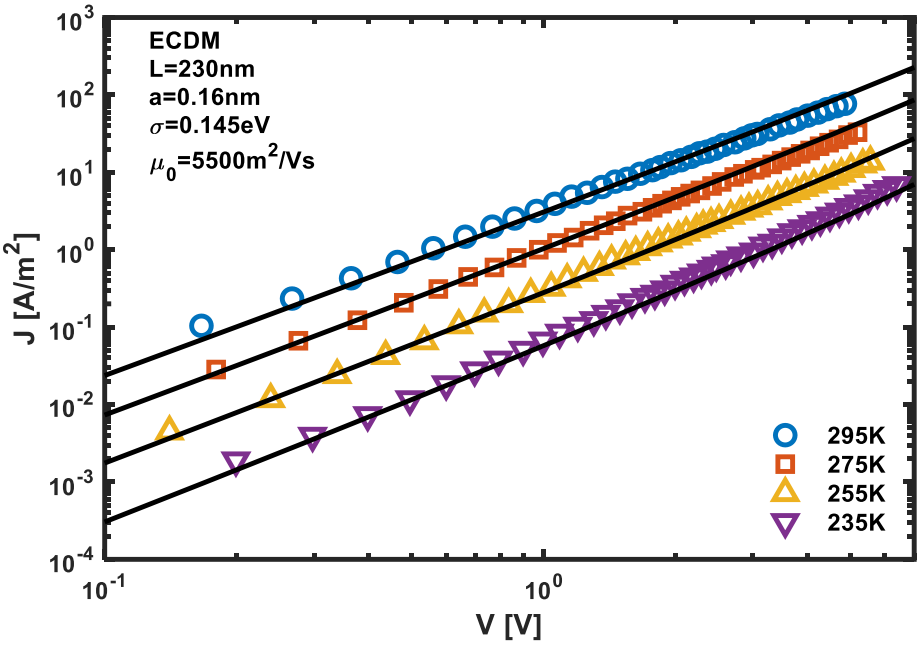

Fig. 4. Temperature dependent J-V characteristics of PFO hole-only device. Symbols are experimental data from Ref. [31]. Lines are the numerically calculated results from the ECDM (colour online)

We further consider the question whether the ET-EGDM model can also provide a consistent description of the hole transport in PFO. Fig.5 and Fig.6 show the thickness and temperature dependent $J-V$ curves of the PFO hole-only devices from the ET-EGDM model. It can be seen from the figures that the thickness and temperature dependent $J-V$ characteristics of PFO hole-only devices can also be excellently described only using a single set of parameters, a =0.7 nm, σ =0.12 eV, and μ_0 =1.2 m^2/Vs. It is clear that the calculated results from the ET-EGDM are in good agreement with experimental data. As for the parameters, the extracted disorder values of σ for the ET-EGDM and EGDM are rather similar. However, the extracted average intersite distance value of a from the ET-EGDM is obviously smaller than that from the EGDM, indicating that the ET-EGDM predicts much stronger electric field E dependence than the EGDM.

These results show that the influence of effective temperature T_{eff} on the charge transport is important, indicating that the effective temperature responsible for the combined effects of the electric field and real temperature on the mobility.

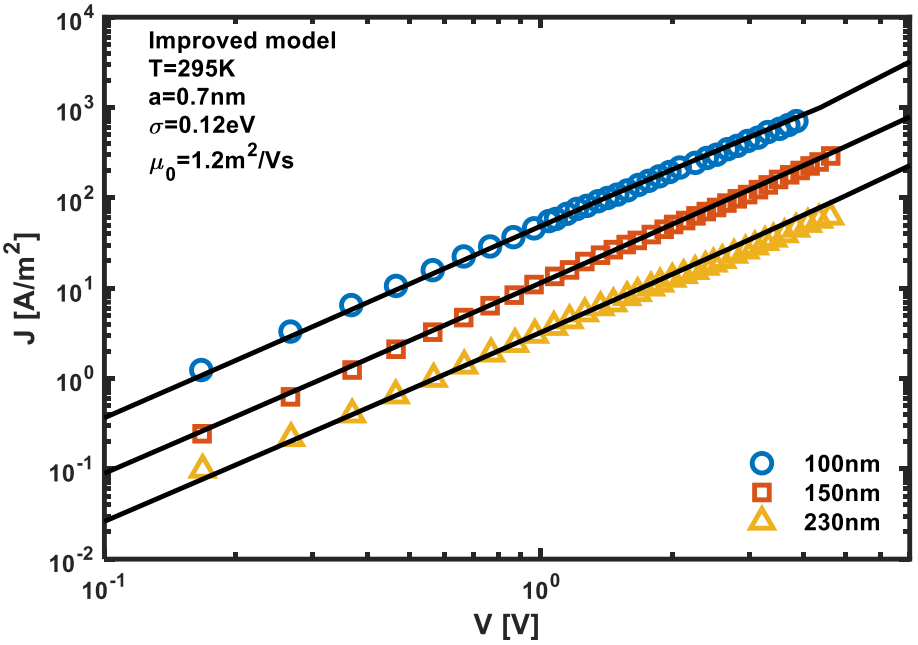

Fig. 5. Thickness dependent J-V characteristics of PFO hole-only devices. Symbols are experimental data from Ref. [31]. Lines are the numerically calculated results from the ET-EGDM (colour online)

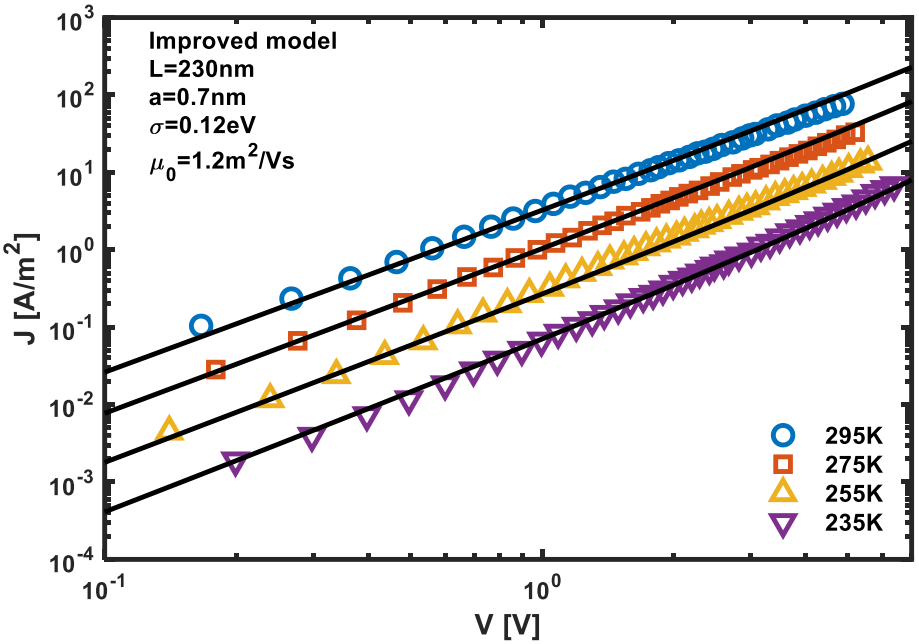

Fig. 6. Temperature dependent J-V characteristics of PFO hole-only device. Symbols are experimental data from Ref. [31]. Lines are the numerically calculated results from the ET-EGDM (colour online)

It can be seen from Figs.1-6 that the EGDM, ECDM, and ET-EGDM models excellent fits to the thickness and temperature dependent $J-V$ characteristics of the PFO hole-only devices can be obtained. There is no significant difference in the fit quality from the three models. The key parameters in these models are the strength of the energetic disorder, quantified by the width of the DOS σ, and the average hopping site distance a. The values of σ obtained from the three models (0.13 ev for the EGDM, 0.145 ev for the ECDM and 0.12 ev for the

ET-EGDM) are rather similar and typically observed to fall in the range 0.06-0.16 eV (typical values of σ for organic semiconductors). It is thus clear that the optimal values of σ obtained from the three models in the present study are physically realistic. However, the extracted values of average intersite distance a from the three models are quite different. The value of a obtained from the ECDM (0.16 nm) may be considered as unrealistically small (significantly lower than the typical value of organic semiconductors, 1 nm). This suggests that for PFO the energies of the sites in between which hopping takes place are uncorrelated. The value of a obtained from the ET-EGDM (0.7 nm) is very close to the typical value (1 nm), and is obviously smaller than that from the EGDM (2.1 nm), indicating that the ET-EGDM predicts much stronger electric field E dependence than the EGDM. As mentioned previously, the EGDM has been heavily criticized for giving an underestimation of the field dependence of the mobility. As we have already known, the lower value of σ can be mainly attributed to the omission of the carrier density p dependence, whereas the higher value of a can be mainly attributed to the underestimation of the electric field E dependence. These results show that the ET-EGDM is suitable to study the charge transport in disordered organic semiconductors, and provides an appropriate description of the field dependence of the mobility.

4. Summary and conclusions

In conclusion, the hole transport in blue-emitting polymer PFO has been investigated. It is found that consistent descriptions with equal quality for the thickness and temperature dependent $J-V$ characteristics of the PFO hole-only devices can be obtained by using the EGDM, ECDM, and ET-EGDM. The extracted values of the width of the Gaussian density of states σ from the three models are rather similar and observed to fall in the range of typical values. However, the average intersite distance a from the ET-EGDM is very close to the typical value of organic semiconductors, and is more realistic than that from the EGDM and ECDM, indicating that the ET-EGDM can provide a more appropriate description of the electric field dependence of the mobility than the EGDM and ECDM.

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