Field and temperature dependence of charge transport in ternary organic solar cells

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In this paper, we present an improved mobility model for charge transport in organic semiconductors by inserting the field dependent effective temperature instead of the real temperature into the temperature dependence of the mobility. The consistent descriptions with equal quality for the temperature and composition dependent current density-voltage characteristics of the hole-only devices based on TQ1:$PC_{71}BM$:$IC_{60}BA$ ternary blends can be obtained by using the extended Gaussian disorder model (EGDM) and our improved model, respectively. However, the extracted values of average intersite distance a from the two models are quite different. The values of a from our improved model are very close to the typical value of organic semiconductors, and are obviously smaller than that from the EGDM, indicating that our improved model can provide a more appropriate description of the electric field and temperature dependence of the mobility than the EGDM.

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1. Introduction

Organic solar cells (OSCs) are potentially key contributors to the next-generation photovoltaics for sustainable and environmentally friendly energy sources [1-5]. In the past few years, bulk heterojunction (BHJ) OSCs have attracted much attention as they offer the possibility to achieve high power conversion efficiency (PCE) [6-8]. This is due to the opportunities offered for easy processing of the active layer and the mixture of organic materials readily soluble in various solvents. The latter brought into conception the ternary blend OSCs. The ternary blend OSCs differ from the well-known binary blend OSCs by one additional component in the mixture of their active layer. This means one can migrate from a donor:acceptor (D:A) binary system to either a D:A:A or a D:D:A ternary system [9-11]. The ternary blends have helped achieve over the last few years a high PCE via enhanced absorption and increased fill factor. This improvement in PCE is not only limited to electronic effects, but also be a positive structural effect. Thus, the third component could also enhance the nanomorphology of the active layer to help in better charge dissociation and transport. Thus, an understanding of charge transport in ternary blends is very important to design and synthesize better materials that can further improve the performance of BHJ OSCs [12-14].

Various models for calculating the charge mobility of organic semiconductors have been proposed in the past few years [15-23]. The Gaussian disorder model (GDM) proposed by Bässler et al. using kinetic Monte Carlo simulations with Gaussian densities of states (DOS) to describe the stochastic energies [15, 16]. The correlated disorder model (CDM) has been proposed by assuming that the interactions of the charge and the dipole give rise to an energy correlation [17]. Afterwards, a strong dependence of the mobility on the carrier density was found, and the Extended Gaussian Disorder Model (EGDM) and Extended Correlated Disorder Model (ECDM) were proposed on the basis of the GDM and CDM [18-20]. The EGDM and ECDM are sometimes considered universal, and are the basis for commercially available organic devices simulation software [12, 21]. However, the methodology to derive the EGDM and ECDM has been heavily criticized for giving an inappropriate description of the electric field and temperature dependence of the mobility [24-26]. Recently, it has been shown that when an electric field is applied to a semiconductor at a finite temperature, the combined effect of the electric field and temperature can be described by the effective temperature [27, 28].

In this paper, to better describe charge transport in organic semiconductors, we present an improved mobility model by adopting the field-dependent effective temperature instead of the actual temperature into the EGDM. From an analysis of the temperature and composition dependent current density-voltage ($J-V$) characteristics of the hole-only devices based on TQ1:$PC_{71}BM$:$IC_{60}BA$ ternary blends, it is found that consistent descriptions with equal quality can be obtained within the improved model and EGDM. However, more realistic values of average intersite distance are obtained

within the improved model than within the EGDM. It is shown that the improved model provides a better electric field and temperature 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.

2. Models and methods

Charge transport in organic semiconductors is due to incoherent hopping of charge carriers between localized states that are randomly distributed in space. The most popular theoretical model to describe charge transport is the Gaussian disorder model (GDM), according to which localized states have a Gaussian energy distribution [15, 19, 24, 26].

$$g(\varepsilon) = \frac{N}{\sigma\sqrt{2\pi}} \exp\left(-\frac{\varepsilon^2}{2\sigma^2}\right) \tag{1}$$

where σ is the energetic disorder of the density of states (DOS), and N is the concentration of localized states that is related to the mean intersite distance (lattice constant) by $a = N^{-1/3}$.

The rates for carrier transitions between localized states are usually described by the Miller-Abrahams expression [29]:

$$V_{ij} = \nu_0 \exp\left(-\frac{2R_{ij}}{\alpha} - \frac{|\varepsilon_i - \varepsilon_j| + |\varepsilon_i - \varepsilon_F| + |\varepsilon_j - \varepsilon_F|}{2k_BT}\right) \tag{2}$$

where α is the localization length of charge carriers in the localized states, ε_i and ε_j are the carrier energies on the starting site i and the target site j, respectively, k_B is the Boltzmann constant, ε_F is the Fermi energy, T is the temperature and R_{ij} is the distance between sites i and j, the prefactor ν_0 is the attempt-to-escape frequency.

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 [19]. This model is often referred to as the EGDM. In the EGDM the mobility can be expressed as

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

$$\mu_0(T) = \mu_0 b_1 \exp(-b_2\hat{\sigma}^2), \tag{4}$$

$$f(T,E) = \exp\left\{0.44\left(\hat{\sigma}^{3/2} - 2.2\right)\left[\sqrt{1 + 0.8\left(\frac{eaE}{\sigma}\right)^2} - 1\right]\right\}. \tag{5}$$

$$\delta \equiv 2\frac{\ln(\hat{\sigma}^2 - \hat{\sigma}) - \ln(\ln 4)}{\hat{\sigma}^2}, \quad \mu_0 \equiv \frac{a^2\nu_0 e}{\sigma} \tag{6}$$

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. The EGDM is considered universal and is the basis of commercially available organic devices simulation software [12, 21]. However, the methodology followed to derive the EGDM parametrizations has been heavily criticized for giving an inadequate description of the field and temperature dependence of the mobility [24-26].

The temperature dependence of the mobility given by the EGDM has the non-Arrhenius form:

$$\mu(T) = \mu_0 \exp\left[-C\left(\frac{\sigma}{k_BT}\right)^2\right], \tag{7}$$

However, it has been known that the non-Arrhenius temperature dependence plays a more important role for the charge transport for the case of low carrier concentrations. At high carrier concentrations, the temperature dependence of the mobility should be determined by Arrhenius law [30, 31]:

$$\mu(T) = \mu' \exp\left(-\frac{\Delta}{k_BT}\right), \tag{8}$$

with Δ the activation energy.

Furthermore, Shklovskii and successors have shown that the combined effects of the electric field and temperature on the mobility can be expressed in the form of an effective temperature [32, 33]:

$$T_{eff} = \left[T^2 + \left(\gamma\frac{eE\alpha}{k_B}\right)^2\right]^{1/2} \tag{9}$$

with $\gamma \approx 0.67$. The validity of the approach based on the effective temperature has been confirmed in numerous studies [24-28].

In principle, Eq. (9) 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}. Based on these results, we propose an improved expression of the temperature dependent mobility based on both the Arrhenius and non-Arrhenius temperature dependence. Furthermore, in order to describe the combined effects of electric field and temperature on the mobility, we will use the field dependent effective temperature T_{eff}, instead of the real temperature T, into the temperature dependence of the mobility. The dependence of the mobility μ on the electric field E, temperature T, and carrier density p

can be described as follows:

$$\mu(T, p, E) = \mu(T_{eff}, p)^{g(T_{eff},E)} \exp[c_1(g(T_{eff}, E) - 1)], \quad (10)$$

$$\mu(T_{eff}, p) = \mu_0(T_{eff}) \exp[\frac{1}{2}(\hat{\sigma}^2 - \hat{\sigma})(2pa^3)^{\delta}], \quad (11)$$

$$g(T_{eff}, E) = [1 + c_2(Eea / \sigma)^2]^{-1/2}, \quad (12)$$

$$\mu_0(T_{eff}) = \mu_0 c_3 \hat{\sigma}^{\lambda} \exp(-\frac{E_{crit}}{k_B T_{eff}} - c_4\hat{\sigma}^2), \quad (13)$$

$$\delta \equiv 2\frac{\ln(\hat{\sigma}^2 - \hat{\sigma}) - \ln(\ln 4)}{\hat{\sigma}^2}, \quad \mu_0 \equiv \frac{a^2 \nu_0 e}{\sigma} \quad (14)$$

where $\lambda = 0.4$, $E_{crit} = -0.491$ (λ is the critical exponent, E_{crit} is the critical energy [34]), $c_3 = 0.7 \times 10^{-9}$, $c_4 = 0.51$, c_1 and c_2 are weak density dependent parameters, given by

$$c_1 = d_1 + d_2 \ln(pa^3), \quad (15a)$$

$$c_2 = 116.2 + 8.96 \ln(pa^3), \quad (15b)$$

$$d_1 = 35.66 - 114.34\hat{\sigma}^{-1} + 310.7\hat{\sigma}^{-2} - 283.76\hat{\sigma}^{-3}, \quad (16a)$$

$$d_2 = -0.157 - 0.021\hat{\sigma} + 0.07\hat{\sigma}^2 - 0.0014\hat{\sigma}^3, \quad (16b)$$

3. Results and discussion

In this section, we will apply the EGDM and our improved model as described in section 2 to the hole-only devices based on TQ1:(1-x)$PC_{71}BM$:x$IC_{60}BA$($0 \leqslant x \leqslant 1$) ternary blends, and then compare the dependence of mobility on the electric field and temperature from the two models. To explore charge transport in more detail and evaluate the dependence of mobility on the field and temperature, we investigate the temperature dependent space-charge limited current (SCLC) for the hole-only devices based on TQ1:(1-x)$PC_{71}BM$:x$IC_{60}BA$ ternary blends. For a system with Gaussian disorder, the mobility can be described by the EGDM and our improved model, 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.

In Figs. 1-3, we present the temperature dependent $J-V$ curves and fitting results from the improved model for hole-only devices based on TQ1:$PC_{71}BM$:$IC_{60}BA$ ternary blends with D:A1:A2 compositions of 1:0.3:0.7, 1:0.5:0.5, and 1:0.7:0.3, respectively. As can be seen from these figures, the experimental data can be well described by using the improved model, within which an optimal fit can be obtained using the parameters of a =0.95 nm, σ =0.09 eV, and μ_0 =30 m^2/Vs (1:0.3:0.7); a =1.2 nm, σ =0.085 eV, and μ_0 =250 m^2/Vs (1:0.5:0.5); a =1.02 nm, σ =0.087 eV, and μ_0 =170 m^2/Vs (1:0.7:0.3). For the model parameters, the values of the disorder parameter σ from the improved model are close to the values obtained by Felekidis et al. [11], which are observed to fall in the range 0.06-0.16 eV (typical values of σ for organic semiconductors). The values of average intersite distance a found from the improved model are almost equal to the typical value of organic semiconductors (1 nm).

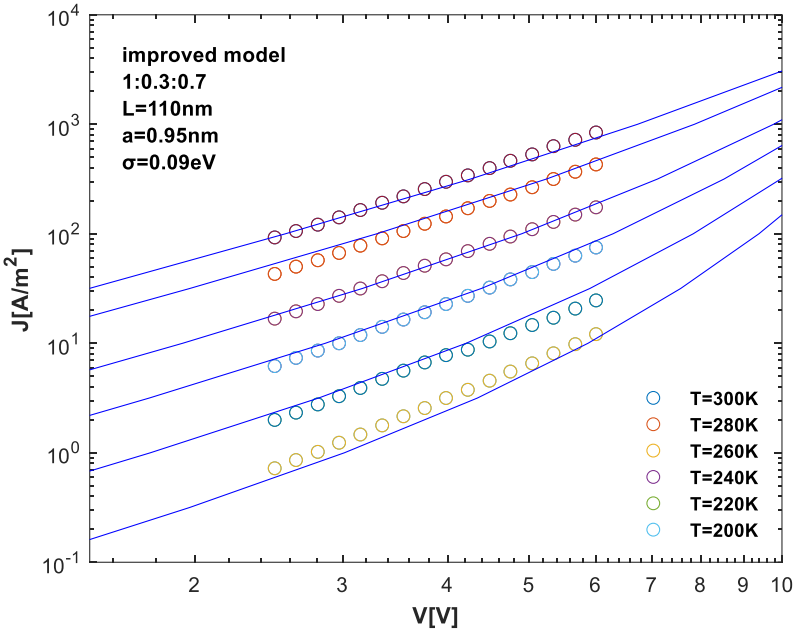

Fig. 1. Temperature dependent J-V characteristics of the hole-only devices based on TQ1:$PC_{71}BM$:$IC_{60}BA$ ternary blends (1:0.3:0.7). Symbols are experimental data from Ref. [11]. Lines are the numerically calculated results from the improved model (colour online)

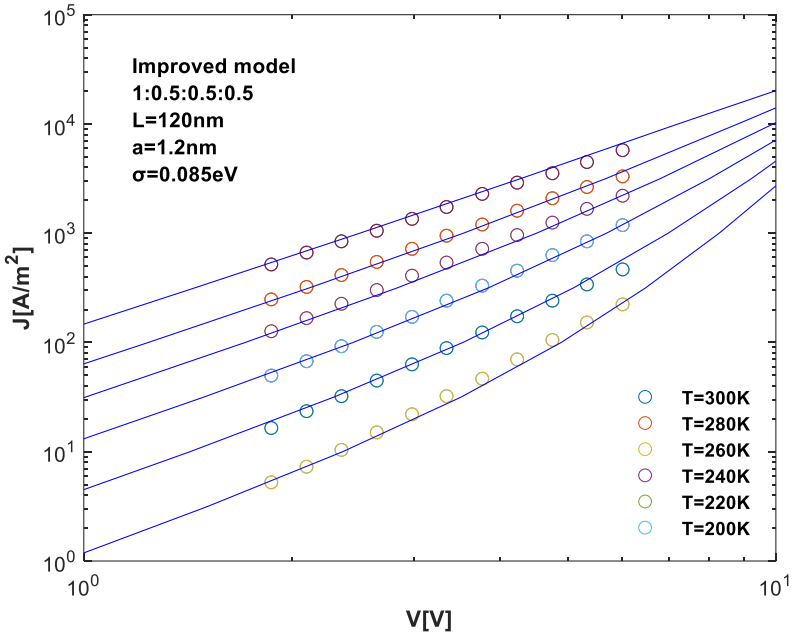

Fig. 2. Temperature dependent J-V characteristics of the hole-only devices based on TQ1:$PC_{71}BM$:$IC_{60}BA$ ternary blends (1:0.5:0.5). Symbols are experimental data from Ref. [11]. Lines are the numerically calculated results from the improved model (colour online)

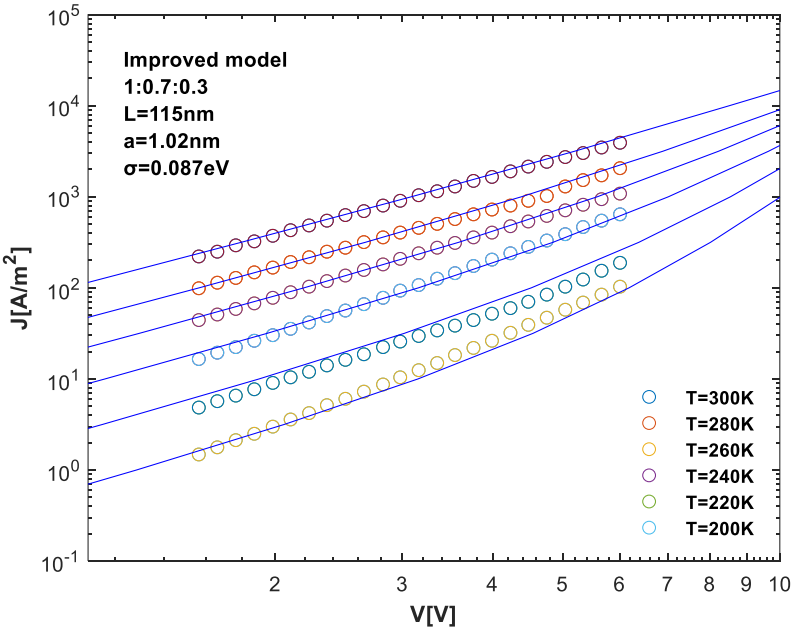

Fig. 3. Temperature dependent J-V characteristics of the hole-only devices based on TQ1:$PC_{71}BM$:$IC_{60}BA$ ternary blends (1:0.7:0.3). Symbols are experimental data from Ref. [11]. Lines are the numerically calculated results from the improved model (colour online)

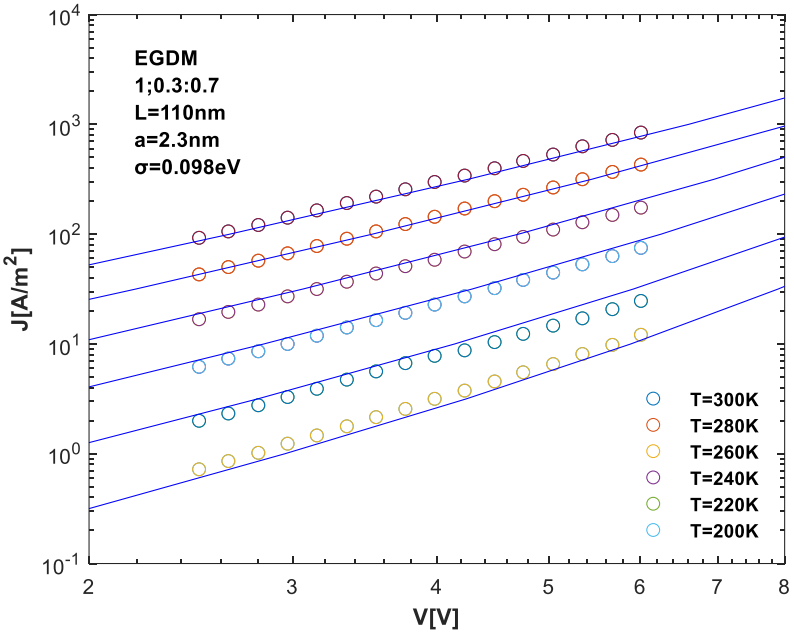

Fig. 4. Temperature dependent J-V characteristics of the hole-only devices based on TQ1:$PC_{71}BM$:$IC_{60}BA$ ternary blends (1:0.3:0.7). Symbols are experimental data from Ref. [11]. Lines are the numerically calculated results from the EGDM (colour online)

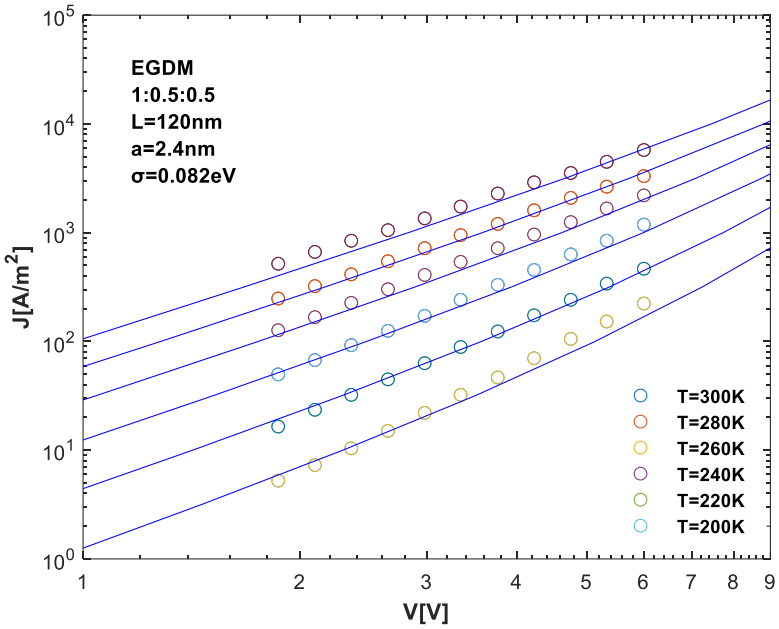

Fig. 5. Temperature dependent J-V characteristics of the hole-only devices based on TQ1:$PC_{71}BM$:$IC_{60}BA$ ternary blends (1:0.5:0.5). Symbols are experimental data from Ref. [11]. Lines are the numerically calculated results from the EGDM (colour online)

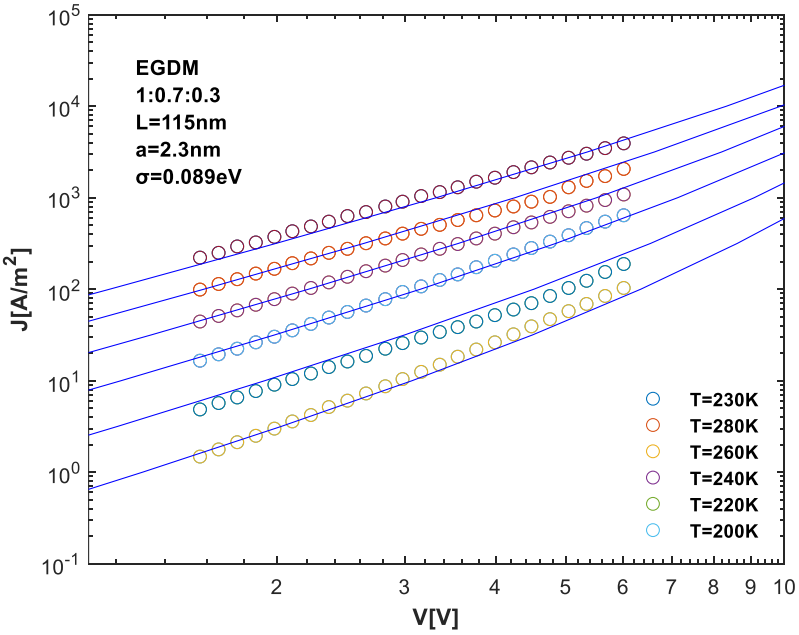

Fig. 6. Temperature dependent J-V characteristics of the hole-only devices based on TQ1:$PC_{71}BM$:$IC_{60}BA$ ternary blends (1:0.7:0.3). Symbols are experimental data from Ref. [11]. Lines are the numerically calculated results from the EGDM (colour online)

As a next step, we now consider the question whether the EGDM can also describe the $J-V$ characteristics of the hole-only devices based on TQ1:$PC_{71}BM$:$IC_{60}BA$ ternary blends. Here, we re-analyse these experimental data for the TQ1:$PC_{71}BM$:$IC_{60}BA$ hole-only devices by using the EGDM. In Figs. 4-6, we present the temperature dependent $J-V$ curves and EGDM fitting results of hole-only devices based on TQ1:$PC_{71}BM$:$IC_{60}BA$ ternary blends with D:A1:A2 compositions of 1:0.3:0.7, 1:0.5:0.5, and 1:0.7:0.3, respectively. Obviously, the temperature dependent $J-V$ curves of the TQ1:$PC_{71}BM$:$IC_{60}BA$ hole-only devices can also be well described within the EGDM by using the parameters of

a = 2.3 nm, σ =0.098 eV, and μ_0 =105 m^2/Vs (1:0.3:0.7); a = 2.4 nm, σ =0.082 eV, and μ_0 =250 m^2/Vs (1:0.5:0.5); a =2.3 nm, σ =0.089 eV, and μ_0 =300 m^2/Vs (1:0.7:0.3). It is found that the EGDM can also provide a good description for hole transport in TQ1:PC_{71}BM:IC_{60}BA ternary blends, provided that a much larger average intersite distance is assumed within the EGDM than the typical value (1 nm). The value of a found from the EGDM may be considered as unrealistically large (significantly larger than the typical value of organic semiconductors).

It can be seen from Figs.1-6 that the EGDM and our improved model excellent fits to the temperature and composition dependent $J-V$ characteristics of the hole-only devices based on TQ1:PC_{71}BM:IC_{60}BA ternary blends can be obtained. There is no significant difference in the fit quality from the two models, but with considerable differences in the model parameters. The key parameters in the two 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 two models 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 two models in the present study are physically realistic. However, the extracted values of average intersite distance a from the two models are quite different. The value of a obtained from the improved model is very close to the typical value (1 nm), and is obviously smaller than that from the EGDM, indicating that the improved model 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 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 temperature on the mobility. Furthermore, it is shown that our improved model is suitable to study the charge transport in disordered organic semiconductors, and provides an appropriate description of the field and temperature dependence of the mobility.

4. Summary and conclusions

In conclusion, the charge transport in hole-only devices based on TQ1:PC_{71}BM:IC_{60}BA ternary blends has been investigated. It is found that consistent descriptions with equal quality for the temperature and composition dependent $J-V$ characteristics of the hole-only devices based on TQ1:PC_{71}BM:IC_{60}BA ternary blends can be obtained by using the EGDM and our improved model. The extracted values of the width of the Gaussian density of states σ from the two models are rather similar and observed to fall in the range of typical values. However, the average intersite distance a from our improved model are very close to the typical value of organic semiconductors, and are more realistic than that from the EGDM, indicating that our improved model can provide a more appropriate description of the electric field and temperature dependence of the mobility than the EGDM.

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