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Electric field-dependent charge transport in organic semiconductors

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An analytical description is elaborated for the variable range hopping conduction mechanism in the presence of temperature and electric fields for quasi-three-dimensional organic semiconductor systems. In the proposed description, it is assumed that the localized states are randomly distributed in energy and space coordinates. The expression for the hopping conductivity is obtained for the Gaussian density of states. The model is applied to the analysis of both temperature and electric field-dependent hopping transport in organic semiconductors. It is shown that the Poole–Frenkel behavior is only valid in medium electric field regime. Moreover, we conclude that the electric field determines whether the temperature dependence of conductivity in organic semiconductors obeys the Arrhenius law. © 2009 American Institute of Physics. [doi:10.1063/1.3246160]

Organic semiconductors, such as conjugated and molecularly doped polymers, represent a rapidly evolving research area due to their current and potential applications in various electronic devices. It is widely accepted that the charge transport in organic semiconductors is governed by variable range hopping (VRH) among a system of localized states.¹ Therefore, the important parameter conductivity (mobility) in such systems is temperature and electric field dependent. Many models have been developed to describe the charge carrier transport in disordered materials systems including empirical Poole–Frenkel model,² temperature-dependent Gill model³ and transport energy model.⁴

However, most of the electric field-dependent charge transport models in organic semiconductors are based on a one-dimensional system description.⁵ Effective temperature model⁶ has also been used for field-dependent charge transport by replacing the temperature by the effective temperature. The physics behind the effective temperature model is not very clear.

In this work, we propose a VRH-based charge transport model in the three-dimensional organic semiconductor system, which gives a field-dependent conductivity (mobility) model. Our model shows that the Poole–Frenkel behavior is not valid for all field regimes. Some recent experiments have demonstrated the non-Arrhenius behavior of mobility in low temperature regime, and claimed that the hopping transport is not suited for organic semiconductors.⁷ In this paper, we show that the hopping transport can also explain the non-Arrhenius temperature characteristics of the mobility in organic semiconductors.

We assume that the localized states are randomly distributed in energy and that space coordinates and the positions of these states, i.e. hopping sites, form a discrete array. This space is called the hopping space. Then, the probability of hopping for a carrier from the initial state i to a final state j in this space is given by⁸

$$W(R) \propto \exp(-R), \quad (1)$$

where R is the distance between these two sites in the hopping space and is called the range.⁸ When there exists an electric field E , the range can be written as

$$R = \begin{cases} R_{ij}(1 + \beta \cos \theta) + \varepsilon_j - \varepsilon_i, & \varepsilon_j > \varepsilon_i - \beta \cos \theta \\ R_{ij}, & \varepsilon_j < \varepsilon_i - \beta \cos \theta. \end{cases} \quad (2)$$

Where $\beta = eE/(2\alpha k_B T)$, R_{ij} is the distance between the two sites, ε_i and ε_j are the energies of sites i and j , e is the elemental charge, α is the decay constant of the assumed hydrogenlike localized states wave functions, and θ is the angle between R_{ij} and the electric field ranging from 0 to π .⁸ The reduced coordinate R_{ij} should be multiplied by $1/2\alpha$ to be expressed in the distance unit. Similarly, ε_i and ε_j should be multiplied by $k_B T$ to comply with the energy units.

Here we assume the a Gaussian density of states (DOS),

$$g(\varepsilon) = \frac{N_t}{\sqrt{2\pi}\sigma^*} \exp\left(-\frac{\varepsilon^2}{2\sigma^{*2}}\right), \quad (3)$$

where N_t is the number of states per unit volume and $\sigma^* = \sigma/k_B T$ indicates the width of the DOS. For a site with energy ε in the hopping space, the most probable hop for a carrier on this site is to an empty site at a range, where it needs the minimum energy. Conduction is the result of a long sequence of hops through this hopping space. Then, following the method in Ref. 8 we derive the number of empty sites enclosed by the constant range R , as

$$N(\varepsilon_i, T, \beta, R) = \frac{1}{8\alpha^3} \int_0^\pi d\theta \sin \theta \int_0^R dr 2\pi r^2 \times \int_{-\infty}^{R+\varepsilon_i-r(1+\beta \cos \theta)} d\varepsilon_j g(\varepsilon_j) [1 - f(\varepsilon_j, \varepsilon_F)]. \quad (4)$$

Here $f(\varepsilon_j, \varepsilon_F)$ is the Fermi–Dirac distribution and $1 - f(\varepsilon_j, \varepsilon_F)$ is the probability that the final site is empty, and the Fermi energy ε_F is calculated by the condition

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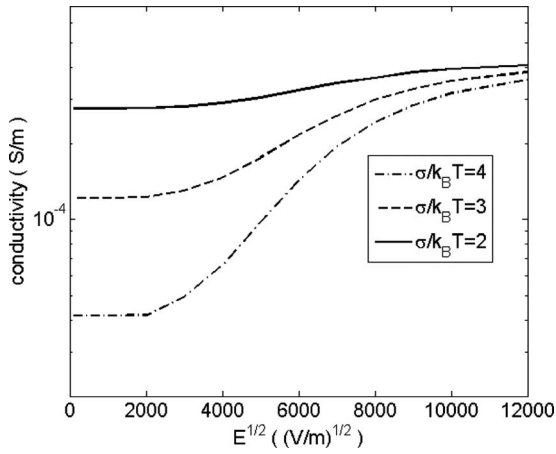


FIG. 1. The field-dependent conductivity at different temperature.

$$n = \frac{N_t}{\sqrt{2\pi}\sigma^*} \int_{-\infty}^{\infty} d\varepsilon \frac{\exp(-\varepsilon^2/2\sigma^{*2})}{1 + \exp(\varepsilon - \varepsilon_F)}, \quad (5)$$

where n is the carrier concentration in organic semiconductors. We assume here that the field shifts both the absolute energy of a site and the Fermi energy at the position of this site; thus the DOS and Fermi distribution shift together, and the occupation probability of a particular site is unchanged.⁸

Based on the VRH theory, the average hopping range $\overline{R(\varepsilon_i)}$ is obtained by setting $N=1$ in Eq. (4). Then the diffusion constant $D(\varepsilon_i)$ is written as

$$D(\varepsilon_i) = \frac{\overline{R(\varepsilon_i)}^2}{6(2\alpha)^2} \nu_0 \exp[-\overline{R(\varepsilon_i)}], \quad (6)$$

where ν_0 is the attempt-to-escape frequency. The conductivity is calculated as⁹

$$\begin{aligned} \sigma_c &= \int_{-\infty}^{\infty} d\varepsilon_i k_B T \frac{e^2}{k_B T} D(\varepsilon_i) f(\varepsilon_i, \varepsilon_F) g(\varepsilon_i) \\ &= \int_{-\infty}^{\infty} d\varepsilon_i e^2 D(\varepsilon_i) f(\varepsilon_i, \varepsilon_F) g(\varepsilon_i). \end{aligned} \quad (7)$$

Finally, the mobility in organic semiconductor is obtained as

$$\mu = \frac{\sigma_c}{ne}. \quad (8)$$

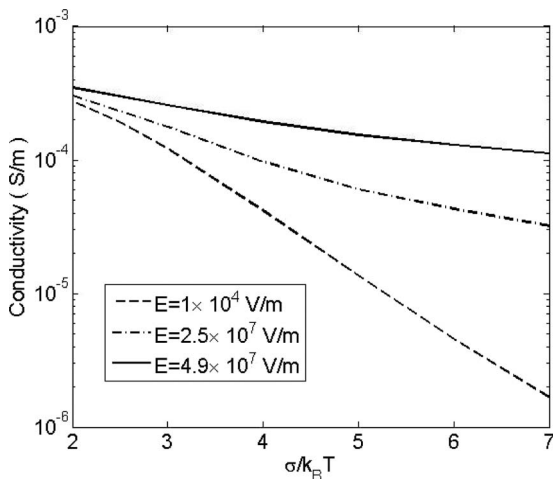


FIG. 2. The temperature-dependent conductivity at different electric field.

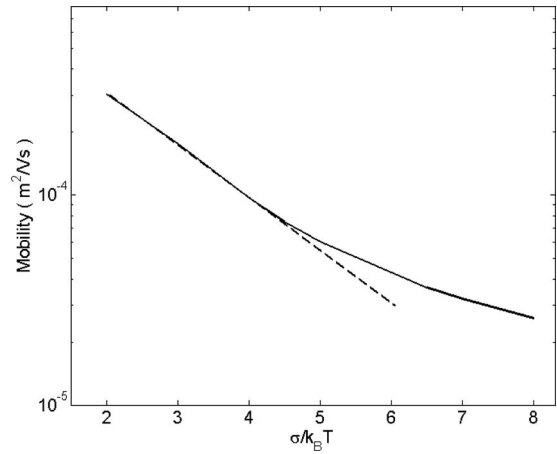
FIG. 3. The temperature-dependent conductivity for $E=2.5 \times 10^7$ V/m.

Figure 1 shows the field-dependent conductivity calculated by Eq. (7). The input parameters are $N_t=1 \times 10^{22} \text{ cm}^{-3}$, $n=1 \times 10^{-4} N_t$, $\alpha^{-1}=1 \text{ \AA}$, and $\nu_0=10^{13} \text{ s}^{-1}$. We can see that, in the low electric field regime, the conductivity remains a constant. When the field increases, the conductivity will increase as well, but the conductivity will saturate when the field is beyond a certain threshold. The empirical Poole-Frenkel form, $\sigma_c \propto \exp(\gamma\sqrt{E})$ (Ref. 2) is only valid for the medium field regime. The temperature dependence of the calculated conductivity is plotted in Fig. 2, where the input parameters are the same as those used in Fig. 1. As can be seen, in the low field regime, the conductivity possesses a perfect Arrhenius relation with the temperature; however, when the electric field is high, the conductivity demonstrates a non-Arrhenius relation in the low temperature regime. The relation between mobility and temperature at $E=2.5 \times 10^7$ V/m is shown in Fig. 3. Clearly, the electric field has a profound impact on the temperature characteristics of the conductivity (mobility). This is because the electric field reduces the energy barrier along the hopping path. As in Ref. 10, we find temperature-independent hopping in the high field regime. The comparison between our model

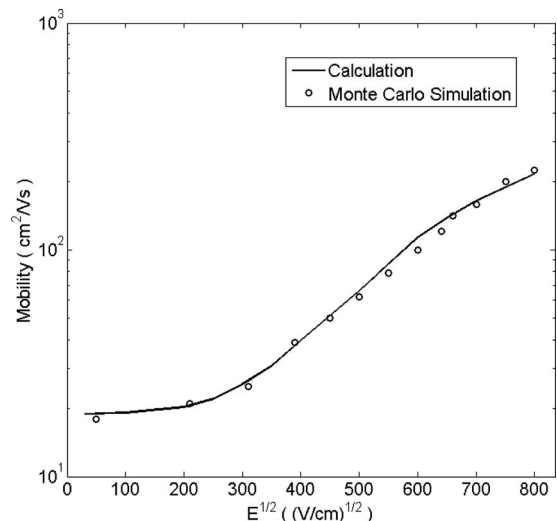


FIG. 4. Comparison between calculation and Monte Carlo simulation.

and the Monte Carlo simulation¹¹ is plotted in Fig. 4, where the input parameters are $\nu_0=10^{10}$ s⁻¹ and $\sigma/k_B T=4.7$. We can observe a good fit between our prediction and the numerical simulations.

To conclude, the hopping conduction mechanism in organic semiconductors has been described analytically. The model is based on the Gaussian DOS and has been applied in the analysis of the role of the field in the hopping transport. We observe that the Pool-Frenkel relation is only valid in the medium field regime and that electric field has an important effect on the temperature dependence of the conductivity (mobility) in organic semiconductors. Good agreement between the model and Monte Carlo simulation is observed.

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