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Influence of traps on charge transport in organic semiconductors

Ling Li *, Gregor Meller, Hans Kosina

Institute for Microelectronics, TU Vienna, Gußhausstraße 27-29, A-1040 Wien, Austria

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Abstract

The effect of extrinsic traps on the charge transport in organic semiconductors has been investigated. An analytical model describing hopping transport with traps is formulated on the basis of percolation theory. The results show that the presence of a trap distribution with energy offset and width different from that of the intrinsic density of states does not change the basic phenomenology of hopping transport, as revealed by the temperature dependence of the conductivity at high temperature. However the traps may significantly affect the transport at low temperature. The relation between trap concentration and conductivity is discussed. The model predictions are in good agreement with experimental results.

Keywords: Traps; Conductivity model; Organic semiconductor; Percolation theory

1. Introduction

Over the past 10 years, the interest in organic semiconductors has increased dramatically. Devices such as organic light emitting diodes and organic field effect transistors have been realized [3,4]. In spite of these successful applications, the physical processes underlying the charge transport in organic semiconductors are not well understood. For example, a proper description of the effect of traps on charge transport is still a challenge. Extrinsic localized states differ from the majority of intrinsic hopping states in disordered media in that they require a substantially larger energy to release charge carrier to the intrinsic density of states (DOS). The Columb potential of trapped carriers will influence the charge transport [5]. Borsenberg studied the effect of traps on charge transport using computer simulation [1]. Arikipov has proposed a model for an effective transport energy for deep trap states. However, a direct proof for the existence such as energy in organic semiconductors is not known [8].

In this article we first derive an analytical expression for the trap-dependent conductivity based on the percolation theory. It is assumed that both intrinsic states and extrinsic traps are distributed with an exponential DOS of different widths, and that both distributions are occupied according to Fermi–Dirac statistics. Then we discuss the effect of traps on the conductivity of organic semiconductors. Finally we compare this model with experimental results.

2. Model theory

In organic semiconductors the transport of carriers is governed by hopping between localized states. The conductivity of such a system can be determined using percolation theory. The system is regarded as a random resistor network as proposed by Miller and Abrahams [9,11]. The current is flowing through bonds connecting the sites of such network. The conductance between the site i and j can be described as [12]

$$s_{ij} = \sigma_0 \exp\left(-2\alpha R_{ij} - \frac{|\epsilon_i - \epsilon_F| + |\epsilon_j - \epsilon_F| + |\epsilon_j - \epsilon_i|}{2k_B T}\right). \quad (1)$$

* Corresponding author.
E-mail address: li@iue.tuwien.ac.at (L. Li).

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Here, σ_0 is a prefactor, α^{-1} is the Bohr radius of the localized wave functions, R_{ij} denotes the distance between the sites i and j, and ϵ_i is the energy of carriers at site i. According to percolation theory [12,13], the critical conductance value s_c determines the conductivity of the system when the first infinite cluster occurs [11].

$$\sigma = \sigma_0 \exp(-s_c). \tag{2}$$

In order to model the influence of traps in a simple manner, we assume a double exponential function for the DOS.

$$g(\epsilon) = \frac{N_t}{k_B T_0} \exp\left(\frac{\epsilon}{k_B T_0}\right)\theta(-\epsilon) + \frac{N_d}{k_B T_1} \exp\left(\frac{\epsilon - E_d}{k_B T_1}\right)\theta(E_d - \epsilon). \tag{3}$$

Here N_t and N_d are the concentrations of intrinsic states and traps states, respectively, θ is the unit step function, T_0 and T_1 are parameters indicating the widths of the intrinsic and the trap state distributions, respectively, and E_d is Coulomb trap energy [14]. Vissenberg and Matters pointed out that they do not expect the results to be qualitatively different for a different choice of $g(\epsilon)$ [13], as long as $g(\epsilon)$ increases strongly with ϵ. Therefore, we assume that transport takes place in the tail of the exponential distribution. The equilibrium distribution of carriers, n, is determined by the Fermi–Dirac distribution as follows

$$\begin{aligned} n &= \int \frac{d\epsilon g(\epsilon)}{1 + \exp\left(\frac{\epsilon - \epsilon_F}{k_B T}\right)} \\ &= N_t \exp\left(\frac{\epsilon_F}{k_B T_0}\right) \frac{\pi T/T_0}{\sin \pi T/T_0} \\ &\quad + N_d \exp\left(\frac{\epsilon_F - E_d}{k_B T_1}\right) \frac{\pi T/T_1}{\sin \pi T/T_1}. \end{aligned} \tag{4}$$

According to the classical percolation theory [12], at the onset of percolation, the critical number B_c can be written as

$$B_c = \frac{N_b}{N_s}, \tag{5}$$

where $B_c = 2.8$ for a three-dimensional amorphous system. N_b and N_s are, respectively, the density of bonds and the density of sites in this percolation system, which can be calculated as follows [13,16]

$$N_b = \int d\mathbf{R}_{ij} d\epsilon_i d\epsilon_j g(\epsilon_i) g(\epsilon_j) \theta(s_c - s_{ij}) \tag{6}$$

$$N_s = \int d\epsilon g(\epsilon) \theta(s_c k_B T - |\epsilon - \epsilon_F|). \tag{7}$$

Here $\mathbf{R}_{ij}$ denotes the distance vector between sites i and j.

Substituting (4), (6) and (7) into (2), we obtain the expression

$$B_c = \frac{\pi N_t^2 \psi^3 \exp(2\eta) + \pi N_d^2 \xi^3 \exp(2\gamma) + \frac{\pi}{4} N_t N_d \exp(\eta + \gamma)(\psi^{-1} + \xi^{-1})^{-3}}{N_t \exp(\eta) + N_d \exp(\gamma)} \tag{8}$$

with

$$\eta = \frac{\epsilon_F + k_B T s_c}{k_B T_0}, \quad \gamma = \frac{\epsilon_F - E_d + k_B T s_c}{k_B T_1},$$
$$\psi = \frac{T_0}{2\alpha T}, \quad \xi = \frac{T_1}{2\alpha T}.$$

This equation is obtained under the following conditions:

- the site positions are random,
- the energy barrier for the critical hop is large,
- and the carrier concentration is very low.

The exponent s_c is obtained by a numerical solution of (8) and the conductivity can be calculated using (2). This model was initially proposed in [15], where a doping level E_d above the intrinsic level E_i was assumed. In the present work, we assume a trap level below the intrinsic level to study the effect of extrinsic traps on the conductivity of organic semiconductors.

3. Results and discussion

Figs. 1 and 2 illustrate the temperature dependence of the carrier conductivity for different trap concentrations. The parameters are $N_t = 10^{22}\,\mathrm{cm}^{-3}$, $E_d = -0.67$ eV, $T_0 = 800$ K, $T_1 = 400$ K, $\alpha = 5\,\mathrm{nm}^{-1}$ and $\sigma_0 = 1 \times 10^4$ S/cm. Despite the effect of the traps, we can see an almost perfect Arrhenius-type temperature dependence in Fig. 1, with the slope affected by the trap concentration. Increasing the latter, the activation energy decreases. In Fig. 2, $\log\sigma$ versus T^{-2} is plotted. The deviation from a straight line occurs at higher temperature, where nearly all carriers occupy the intrinsic states, and the filled extrinsic trap states do not change the trap-free hopping relation $\log\sigma \propto T^{-2}$ [7]. However, at lower temperature, the carrier distribution will be pinned near the peak of trap DOS [6].

In Fig. 3 we compare the analytical model with experimental data reported in [1]. Parameters are the relative

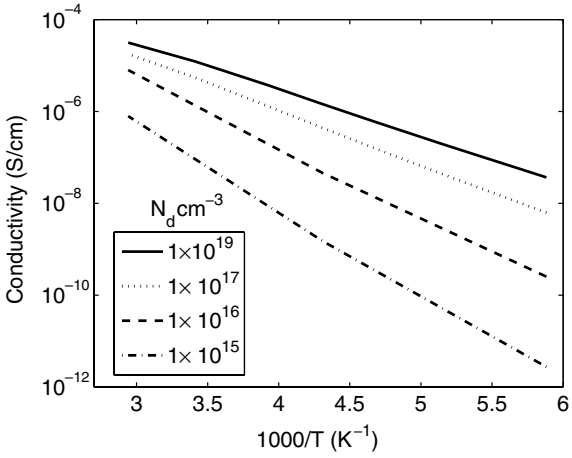

Fig. 1. Conductivity of an organic semiconductor versus T^{-1} for different trap concentrations.