Temperature and Field-dependence of Hopping Conduction in Organic Semiconductors

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After the discovery of electroluminescence in the conjugated polymer PPV [1] and its derivatives, much effort has been devoted to the study of the (opto)electronic and electrical transport properties. Understanding the charge-carrier transport properties in these organic materials is of crucial importance to design and synthesize better materials and to improve device performances. Two of the most important parameters are conductivity and mobility of the charge carriers. In particular, the dependence of conductivity on temperature and electric field has been extensively studied in various papers [2, 3, 4]. The traditional approach to the analysis of the temperature dependence in disordered organic systems is based on the Miller-Abrahams expression [3]. The electric-field dependence in such systems shows Poole-Frenkel behavior $\ln \mu \propto \exp(\gamma \sqrt{E})$ [2]. However, a mechanism is needed to explain such behavior of conduction. This led to a more systematic derivation of the temperature dependence based on the variable range hopping (VRH) and percolation theory [5, 6]. Although the VRH theory has been applied successfully to describe the temperature dependence of conductivity in organic materials, it is difficult to account for the experimentally observed electric field dependence.

In this work, we extend the VRH theory to get a temperature and electric-field dependent conductivity model. The model shows good agreement with experimental data.

For a disordered organic semiconductor system, when an electric field $\vec{F}$ exists, the transition rate of a carrier hopping from site i with energy E_i to the site j with the energy E_j is described as (when $E_j > E_i$) [7]

$$\omega_{ij} = \gamma \exp\left[-(2\alpha + \beta \cos\theta)R_{ij} - \frac{E_j - E_i}{k_B T}\right] \tag{1}$$

where γ is depending on the phonon spectrum, θ is the angle between $\vec{F}$ and R_{ij}, $\beta = eF/(k_B T)$, e is the electrons charge and R_{ij} is the distance between the two sites i,j. When $E_j < E_i$, $\omega_{ij} = \gamma \exp(-2\alpha R_{ij})$. Applying (1), the current between the two sites is given by [7]

$$I_{ij} = \gamma \exp\left[-(2\alpha + \beta \cos\theta)R_{ij} - \frac{|E_j - E_i|}{2k_B T}\right] \sinh\left(\frac{\mu_j - \mu_i}{2k_B T}\right) \left[\cosh\left(\frac{E_i - \mu_i}{2k_B T}\right)\cosh\left(\frac{E_j - \mu_j}{2k_B T}\right)\right]^{-1} \tag{2}$$

Here α^{-1} is the Bohr radius of the localized wave function, μ_i μ_j are the chemical potentials at the positions i and j. According to percolation theory [5], the conductivity of an organic semiconductor system is given by $\sigma = \sigma_0 e^{-s_c}$, where σ_0 is a prefactor and s_c is the exponent of the critical percolation conductance. Assuming that most carriers occupy the sites with energy $\epsilon \ll 0$ and the maximum energy hop is large, we obtain

$$\sigma = \sigma_0 \left\{ \frac{4\pi k_B \delta N_t}{\eta eF B_C} \frac{T_0^3}{T^3} \frac{1}{\Gamma(1 - T/T_0)\Gamma(1 + T/T_0)} \left[\left(2\alpha - \frac{\eta eF}{2k_B T}\right)^{-2} - \left(2\alpha + \frac{\eta eF}{2k_B T}\right)^{-2}\right]\right\}^{T_0/T} \tag{3}$$

where δN_t is the density of charge carriers, B_c is the critical number of bonds per site, η is a parameter for chemical potential and T_0 is a measure for the width of the exponential density of states. To describe the mobility, we use $\mu = \Delta\sigma/(eP)$, where P is the induced carriers concentration, to obtain the field-effect mobility as [8]

$$\mu = \sigma(\delta, T)\frac{T_0}{T}\frac{1}{q\delta N_t}. \tag{4}$$

We use the presented model to calculate the temperature and electric field characteristics of the conductivity of organic semiconductors. In Fig.1, the curves are obtained from (3) using $\sigma_0 = 12.5 \times 10^5 S/m$, $T_0 = 485K$ and $\alpha = 2.7 \times 10^{10}$. The temperature-dependence of conduction and mobility according to (4) is depicted in Fig.2. The experimental data is from [8]. At the same time, the conductivity increases as $\ln\sigma \propto E^{1/2}$ (see Fig.3) with the electric field. The curve is obtained from (3).
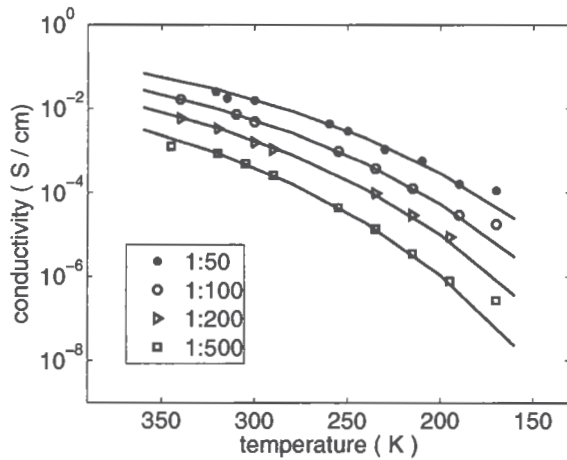
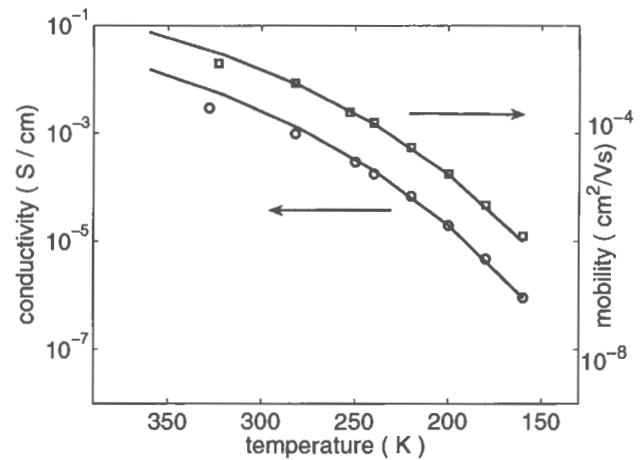**Figure 1:** Conductivity versus temperature at different doping ratio.

Figure 2: Conductivity and mobility versus temperature .

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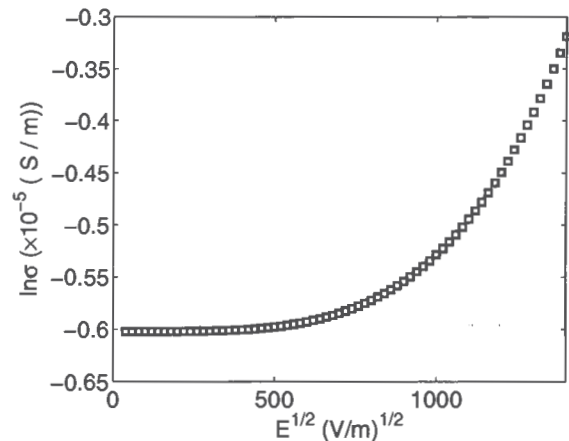
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Figure 3: The electric field dependence of conductivity.