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Percolation Current in Organic Semiconductors

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INTRODUCTION

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 carrier transport properties in these organic materials is of crucial importance to design and synthesize better materials and to improve device performances. The electrical transport in organic semiconductors has been widely investigated for several decades in theoretical as well as experimental studies [2], [3], [4], [5]. For the important concept of variable range hopping (VRH) [6] it is difficult to account for the electric field characteristics observed by experiments.
In this work, we extend VRH theory for organic semiconductors to include percolation theory [7]. The developed model shows good agreement with Mott's formalism at high electric field.

MODEL

For a disordered organic semiconductor system, when an electric field F exists, the transition rate of a carrier hopping from site i with energy E_i to site j with energy E_j is described as [8]

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

and

$$\omega_{ij} = \gamma \exp\left(-2\alpha R_{ij}\right) \quad (E_j \leq E_i + \beta\cos\theta R_{ij})$$

where γ is dependent on the phonons spectrum, α^{-1} is the Bohr radius of the localized wave function, k_B is the Boltzmann constant, $\beta = eF/(k_B T)$, e is the electrons charge, R_{ij} is the distance between the two sites i and j, and θ is the angle between F and R_{ij}. Assuming no correlation between occupation probability of different localized states, the current between the two sites is given by

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

where

$$\zeta = \sinh\left(\frac{\mu_j - \mu_i}{2k_B T}\right) \times \left[\cosh\left(\frac{E_i - \mu_i}{2k_B T}\right)\cosh\left(\frac{E_j - \mu_j}{2k_B T}\right)\right]^{-1}$$

In this model, it is assumed that both the backbone of the percolation cluster and the threshold current do not alter upon rearranging the site potentials. At the same time, the redistribution of the charge seems negligible due to the large spread in I_{ij} at the high electric field.
We consider a network of sites connected with impedances proportional to I_{ij}^{-1}. According to general percolation theory, the critical percolation cluster of sites would comprise a current carrying backbone with at least one site-to-site current equal to the threshold value. As shown in [9], optimization of the current is obtained when the site potentials are altered in such a way that the single hopping event with smallest tunneling probability is optimized. With these assumptions, we can get the equation

$$B_c \approx N_t \frac{2\pi k_B T \xi}{3qF\delta} S_c^3 \eta \quad (2)$$

with

$$\xi = 1 - \frac{\delta}{\Gamma\left(1 - T/T_0\right)\Gamma\left(1 + T/T_0\right)}$$

$$\eta = \left(2\alpha - \frac{eF}{2k_B T}\right)^{-2} - \left(2\alpha + \frac{eF}{2k_B T}\right)^{-2}$$

B_c is the critical number of bonds per site, Γ is gamma function, δ is carrier occupation [10], N_t is the number of states per unit volume, S_c is

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the exponent of the critical percolation current $I = I_0 \exp(-S_c)$, and T_0 is the width of the exponential density of states. This yields an expression for the current in organic semiconductors as a function of the electric field

$$I = I_0 I_t = I_0 \exp\left[-\left(\frac{3eFB_c}{N_t \pi k_B T \xi \eta}\right)^{1/3}\right] \quad (3)$$

where I_0 is a prefactor and I_t is the critical current.

RESULTS AND DISCUSSION

We use the present model to calculate the electric field characteristic of the percolation current in organic semiconductors, as shown in Fig.1. Clearly, the expected dependence that $\log I \sim F^{-1/4}$ is observed at high electric field, the comparison with Mott formalism

$$I_t \sim \exp\left(-\left(C_F \alpha^4 / eN_t F\right)^{1/4}\right)$$

is also provided, Mott formalism can be seen as the asymptote of our model. The input parameters are $N_t = 10^{19} cm^{-3}$ and $T_0 = 380$ K. In Fig.2 we provide the temperature dependence of the percolation current. It can be seen that temperature plays a minor role in hight electric field current.

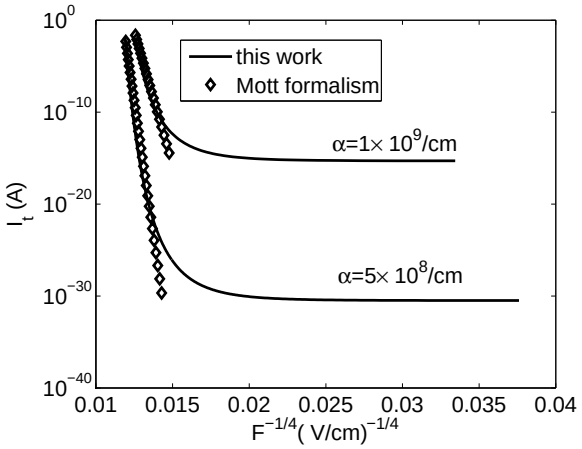

Fig. 1. Electric field dependence of percolation current in a network of localized states.

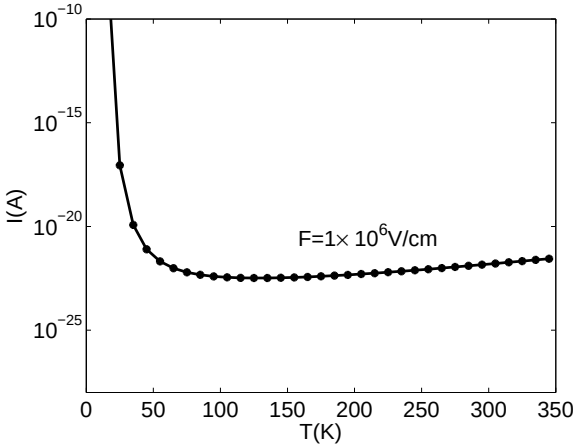

Fig. 2. Temperature dependence of percolation current in a network of localized states in the high electric field regime.

CONCLUSION

We developed an analytic model of high electric field current applicable for organic semiconductors. This model is shown to agree with Mott's formalism. We also discussed the temperature characteristics of this model.

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REFERENCES

[1] J. H. Burroughes, D. Bradley, A. Brown, R. Friend, P. Burn, and A. Holmers, "Point defects and dopant diffusion in silicon," *Nature*, vol. 347, pp. 539–541, 1990.

[2] P. M. W. Blom, M. J. M. de Jong, and M. G. van Munster, "Electric-field and temperature dependence of the hole mobility (p-phenylene vinylene)," *Phys. Rev. B*, vol. 55, no. 2, pp. 656–659, 1997.

[3] W. D. Gill, "Drift mobilities in amorphous charge-transfer complexes of trinitrofluorenone and poly-n-vinylcarbazole," *J. Appl. Phys*, vol. 43, no. 12, pp. 5033–5040, 1972.

[4] A. Miller and E. Abrahams, "Impurity conduction at low concentrations," *Phys. Rev*, vol. 120, no. 3, pp. 745–755, 1960.

[5] P. M. Anderson, "Absence of diffusion in certain random lattices," *Phys. Rev*, vol. 109, pp. 1492–1505, 1958.

[6] N. F. Mott, "Conduction in noncrystalline materials. iii localized states in pseudogap and near extremities of conduction and valence bands," *Philos. Mag*, vol. 19, pp. 835–852, 1969.

[7] V. Ambegokar, "Hopping conductivity in disordered system," *Phys. Rev. B*, vol. 4, no. 8, pp. 2612–2620, 1971.

[8] M. Pollak and I. Riess, "A percolation treatment of high-field hopping transport," *J. Phys. C*, vol. 9, pp. 2239–2352, 1976.

[9] J. van Hapert, *Hopping conduction and chemical structure: a study on silicon suboxides*. PhD thesis, University Utrecht, Netherlands, 2002.

[10] M. C. J. M. Vissenberg and M. Matters, "Theory of the field-effect mobility in amorphous organic transistors," *Phys. Rev. B*, vol. 57, no. 20, pp. 12964–12967, 1998.