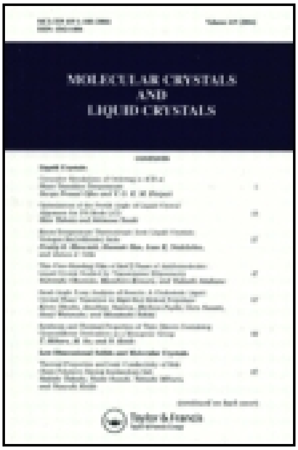

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Charge Carrier Transport in Nonpolar Disordered Organic Materials: What is the Reason for Poole-Frenkel Behavior?

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Recently it was found that the mobility field dependence in disordered organic materials is closely connected with the spatial decay of the energy correlation function. For example, a dipolar glass produces a correlation function decaying as inverse distance, thus leading to a well-known Poole-Frenkel (PF) field dependence. From this point of view a frequent experimental observation of the PF dependence in nonpolar organic materials cannot be explained. We show that the model of quadrupolar glass which is suitable to describe transport properties of nonpolar materials produces a field dependence that is very close to the PF one if measured in not very wide field range. Dispersive effects bring this dependence even more close to the PF one.

Keywords: nonpolar organic materials; charge carrier transport

Until recently, a widely accepted Gaussian Disorder Model (GDM) was considered as giving essentially adequate picture of the hopping charge carrier transport in disordered organic materials. According to the

GDM, charge transport occurs as a series of carrier hops between localized states with energies having Gaussian distribution.[1] The most significant parameter of the theory - energy variance σ^2 - describes contributions from all types of disorder in the uniform way that does not depend on the particular kind of disorder. Hence, in the GDM different kinds of disorder (disorders of different nature) are indistinguishable. Recent results show that this is not true and results of the GDM are directly applied only to the case of totally uncorrelated distribution of transport sites' energies.

According to the new paradigm of the hopping charge carrier transport in disordered organic materials, the mobility field dependence in particular material is directly related to the spatial dependence of the energy correlation function.[2-4] For example, a dipolar glass produces a correlation function that is proportional to the inverse distance, thus leading to a well-known Poole-Frenkel field dependence.[2,3] In general, the 1D model predicts that if the correlation function $C(r) \propto 1/r^p$, then $\ln \mu \propto E^n$ with $n = p/(p+1)$.[2]

From this point of view a frequent experimental observation[5-7] of the PF dependence with $n = ½$ in nonpolar organic materials cannot be explained. Indeed, we cannot present a universal mechanism capable to produce correlation function $C(r) \propto 1/r$ for a wide class of nonpolar organic materials.

More thorough consideration reveals, however, that in such materials the experimentally tested field range is not too broad (not significantly greater than one order of magnitude or even less) and, moreover, sometimes clearly visible deviations from straight lines can be observed when $\ln \mu$ is plotted against $E^{1/2}$.[5] In some cases these deviations lead to the upward convexity of the mobility curve, while in others they lead to the downward convexity. Quite formally, this behavior may be described by $\ln \mu \propto E^n$, with n being in some cases smaller than 0.5 and in some cases greater than 0.5. This observation hints that, quite possibly, in nonpolar organic materials the real mobility field dependence is not a true PF dependence, but rather a quasi-PF dependence with $n \neq 0.5$. This quasi-PF dependence can successfully imitate true PF dependence in not so wide field range.

Quasi-PF field dependence arises naturally in the model of quadrupolar glass.[4] This model seems to be a reasonable model for nonpolar organic materials. Typically, organic molecules possess significant quadrupole moments. For quadrupolar glass[4]

$$C_q(\mathbf{r}) = 0.5\sigma_q^2\left(\frac{a}{r}\right)^3, \qquad (1)$$

and a general result of 1D model[2]

$$\mu = \frac{\mu_0 kT}{eE\int_0^\infty dy \exp\left(-eyE/kT + [C(0)-C(y)]/(kT)^2\right)} \qquad (2)$$

gives for the case of strong disorder $\sigma_q/kT >> 1$

$$\ln\mu \propto -\left(\frac{\sigma_q}{kT}\right)^2 + \frac{2^{3/2}}{3^{1/4}}\left(\frac{\sigma_q}{kT}\right)^{1/2}\left(eaE/kT\right)^{3/4}, \qquad (3)$$

where a is a minimal separation between charge carrier and quadrupole (in the case of a lattice model a is a lattice scale). This dependence is close enough to the PF dependence and can successfully imitate it in not so wide field range. We should expect that result of 1D model is quite reliable: for example, for the case of dipolar glass the 1D model predicts[2]

$$\ln\mu \propto -\left(\frac{\sigma_d}{kT}\right)^2 + 2\frac{\sigma_d}{kT}\sqrt{eaE/kT}\,, \qquad (4)$$

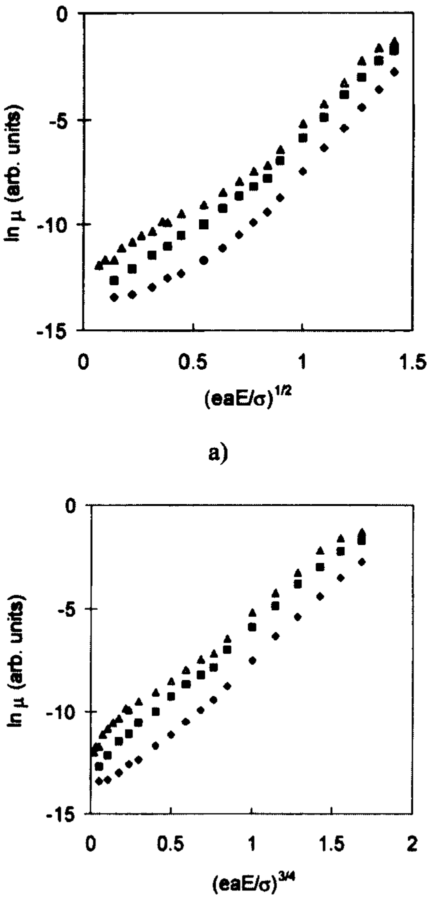
while an accurate computer simulation of 3D transport gives[8]

$$\ln\mu \propto -\left(\frac{3\sigma_d}{5kT}\right)^2 + C_0\left[\left(\frac{\sigma_d}{kT}\right)^{3/2} - \Gamma\right](eaE/\sigma_d)^{1/2} \qquad (5)$$

with $C_0 = 0.78$ and $\Gamma = 2$, so the main difference between (4) and (5) is limited to values of numeric coefficients.

We see that the model of quadrupolar glass indeed produces the mobility field dependence (3) that is very close to the PF dependence. Moreover, we believe that there is an additional reason for the field dependence in nonpolar materials to imitate the PF dependence. This reason is the contribution of dispersive effects. In the case of dispersive transport $\mu \propto E^{\alpha}$,[9] and this dependence, superimposed to the dependence (3), brings it even more close to the PF one. To test this prediction, we carried out a computer simulation of charge transport in 3D cubic lattice with basic sample size of 64×64×64 sites (with periodic boundary conditions applied) occupied by randomly oriented quadrupoles, so the energy of a carrier at a given site is the sum of its interaction with quadrupoles at all sites except its own. If our prediction is valid, we should expect that with the decrease of the transport layer thickness the mobility dependence should go more and more close to the PF dependence. This is indeed the case (see Fig. 1). Note that for the layer with thickness of 100 lattice planes the mobility dependence plotted as $\ln\mu$ vs $E^{3/4}$ is convex upward in small field region, indicating a significant dispersivity of the carrier transport.

In conclusion, we argued that the reasons for the experimental



a)

b)

FIGURE 1 Mobility field dependence for a quadrupolar glass with $kT/\sigma = 0.15$ and different thickness of the transport layer: 100 lattice planes - triangles, 500 planes - squares, and 20,000 planes - diamonds, correspondingly.

observation of the PF field dependence in nonpolar materials are a closeness of the intrinsic field dependence for quadrupolar glass (3) to the PF dependence and contribution of dispersive transport. A possible experimental test for this explanation could be a careful study of the mobility field dependence in wide field range and for thick transport layers, where we should expect deviation from the PF dependence.

Acknowledgments

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