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Correlation Properties of Organic Dipolar Glasses and Charge Carrier Transport in These Materials

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Distribution of the electrostatic potential in dipolar glasses is very strongly spatially correlated. The ultimate reason for this correlation is the long range nature of the dipole's electrostatic potential. Smooth distribution of the electrostatic potential gives significant correlated contribution to the distribution of energy levels of transport centers in dipolar medium and dictates the electric field dependence of carrier drift mobility.

Keywords dipolar glasses, charge carrier transport

INTRODUCTION

Recently it was shown that dipolar glasses have a non-trivial structure in distribution of the electrostatic potential φ, generated by randomly oriented and orientationally non-correlated dipoles. Long range nature of the dipole potential leads to a cluster structure of dipole matrices: sites with close value of electrostatic potential tends to group together[1] (see Fig. 1). The simplest way in which this property manifests itself is a very slow decay of the binary correlation function[1,2]

$$C(\mathbf{r}) = \langle \varphi(0)\varphi(\mathbf{r}) \rangle \propto 1/r, \qquad (1)$$

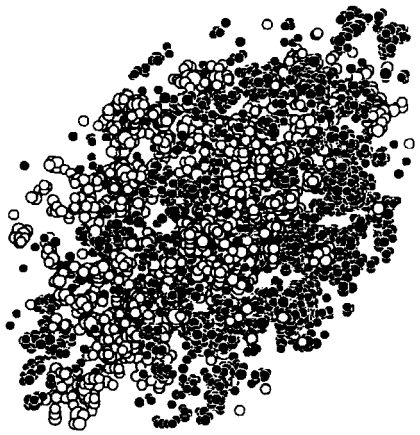

FIGURE 1 Distribution of electrostatic potential in dipolar matrices. Black spheres show sites with positive value of φ, white spheres show sites with negative value of φ, and radius of sphere is proportional to $|\varphi|$.

where angular brackets mean statistic averaging over dipoles orientations and positions. In a typical case the distribution of φ has a Gaussian form,[3] so the dipolar glass is an example of the correlated Gaussian system. In comparison to non-correlated Gaussian system with the same variance, the correlation leads to a significant shift of the percolation threshold and giant increase (up to many orders of magnitude) of the density of large clusters. We found that in dipolar matrix the density of clusters decreases approximately as power law of the cluster size with the exponent close to 1.85 (see Fig. 2).

Electrostatic potential φ gives a significant contribution $E_{dip} = e\varphi$ to the total energy of charge carrier on a typical transport site. We believe that the spatial correlation (1) is the very reason of the Poole-Frenkel (PF) mobility field dependence $\ln \mu \propto F^{1/2}$, which is generally observed in disordered organic materials[4] (here F is the electric field). This fact is confirmed both by the computer simulation of the transport properties of 3D dipolar matrix[5,6] (see Fig. 3) and by the analytical solution for 1D model.[2]

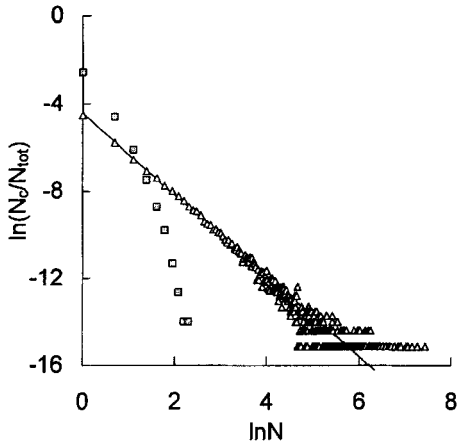

FIGURE 2 Cluster distribution on size (squares - non-correlated Gaussian distribution of the potential, triangles - dipolar matrix with the same variance). Here N is the cluster size (number of sites in a cluster), N_c is the number of clusters and N_{tot} is the total number of sites. Straight line has a slope of -1.85.

Until recently, the most popular model of charge carrier transport in disordered organic materials was the Gaussian disorder model[7] (GDM), where transport occurs as a series of hops between localized states characterized by the Gaussian distribution of site energies without any spatial correlation between energies of different sites. The dipolar model is essentially the correlated version of this model. Effects of correlation remove the major obstacle of the GDM - its inability to explain the PF behavior in low field region (from 10^6 V/cm down to 10^4 V/cm,[4] while in GDM the narrow linear region exists in the field range 3×10^5 - 10^6 V/cm,[7] see also Fig. 3).

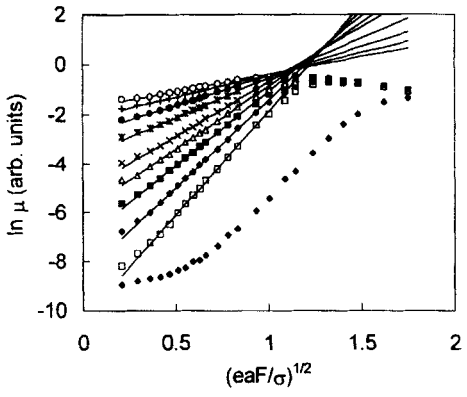

FIGURE 3 Mobility field dependence for different values of σ/kT (from top curve downward): 5.73, 5.10, 4.60, 4.17, 3.82, 3.28, 2.87, 2.55, and 2.30, correspondingly. The lowest curve is the mobility field dependence for GDM for $\sigma/kT = 5.10$. In typical dipolar matrix intersite distance $a \cong$ 10A and variance $\sigma \cong 0.1$ eV,[2,5,6] so $eaF/\sigma \approx 1$ for $F = 10^6$ V/cm.

Computer simulations show that the overall dependence of the mobility on T and F has the form

$$\ln \mu \propto -(\frac{3}{5}\sigma\beta)^2 + C_0\left[(\sigma\beta)^{3/2} - \Gamma\right](eaF/\sigma)^{1/2}. \qquad (2)$$

Here $\sigma^2 = < E_{dip}^2 >$ is the variance of carrier energy and a is the intersite distance. For the regular 3D lattice with every site occupied by dipole $C_0 =$ 0.78 and $\Gamma = 2$. Analogy with GDM suggest that Γ depends on positional disorder and expected to be greater than 2 for disordered organic materials.

To demonstrate use of (2), we present here a comparison with experimental data for NPPDA, a highly polar organic glass[8] with dipole moment $p = 3.02$ D. The temperature dependence of the mobility

extrapolated to zero field gives $\sigma = 0.109$ eV. The temperature dependence of the slope of the mobility field dependence gives $\sigma = 0.095$ eV. The difference is small enough to neglect it completely because of the oversimplified nature of the model (for example, change of C_0 from 0.78 to 0.68 eliminates any difference in σ). Besides, a probable reason for this difference is a contribution from the short range stochastic component to the total energy of the charge carrier on the transport sites (for example, Van der Waals contribution[8]). This contribution has no impact on the PF slope in low field region,[9] but adds an additional term to the temperature dependence of the extrapolated mobility. For the simple cubic lattice[3] $\sigma_{dip} = 2.35\ ep/\varepsilon a^2$, which gives 0.084 eV in reasonable agreement with experimental data. The only significant difference between the simulation and experimental data is the difference in Γ (4.55 instead of 2). We should expect such difference because of the total neglect of the positional disorder in current incarnation of our model.

We considered the correlation properties of dipolar glasses and showed that this very correlation leads to Poole-Frenkel mobility field dependence in disordered organic materials. We compared the transport properties of correlated dipolar matrices with those of non-correlated Gaussian model. The most obvious differences between the models are: 1) much wider region where the PF dependence is valid in the dipolar model and 2) shift of this region to lower electric fields. Both features significantly improve the agreement with the experimental data.

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