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To cite this article: V R Nikitenko and V M Sukharev 2016 *J. Phys.: Conf. Ser.* **741** 012080

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Transport level in disordered organics: correlated energetic disorder in dipole glass model

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Abstract. In this paper Monte-Carlo modeling is in use in order to further approve and quantify the concept of effective transport level in the respect to organic materials with correlated disorder. We consider a model of dipole glass (simple cubic lattice, which sites are occupied by randomly oriented dipoles). Both the absolute values and dependence of the effective transport level on the disorder and temperature, in the limit of low electric field, is very similar to the same in the case of uncorrelated disorder

1. Introduction

Organic optical-electronics devices, such as light-emitting diodes, photovoltaic cells, consist of thin active layers. Predictive modeling of operation of such devices unavoidably needs correct characterization of charge transport in organic layers. The concept of transport level [1] (or transport energy) is known to be a useful tool for analytic modeling, providing uncorrelated Gaussian disorder [2], because it can simplify the description of hopping transport greatly. By the use of transport level concept, which is an analog of mobility edge, mobility of charge carriers can be calculated in analogy with multiple trapping model.

Transport level is neither an energy of final state after the first jump from a deep state nor a most visited energy in course of transport. So one needs to consider random walk of a carrier inside a region of some radius around initial state [1]. Model of dipole glass is the simplest model of disordered organic materials that have polar molecules and where energetic disorder is spatially correlated [2]. Previously, an applicability of effective transport level concept [1] to disordered organics with correlated disorder was shown qualitatively by Monte-Carlo modelling in the framework of the dipole glass model [3]. The purpose of this paper is to test this applicability again by the means of more effective algorithm, quantify the temperature dependence of the effective transport level and compare it with analogous results, which were obtained previously [1] in the framework of uncorrelated Gaussian disorder model [2].

2. Monte-Carlo procedure and scheme of modeling

In MC simulations we use the same approach to the modeling of random walk in disorder media [4], that was applied in our previous works [[5], [6]]. Hopping centers are located at sites of a simple cubic lattice, all sites occupied by dipoles. The whole volume is divided by 3 sub-volumes, see Figure. 1a. A carrier allowed to walk inside the first (the inner) sub volume; energies are calculated also for any state of the second sub volume, which is necessary to evaluate probabilities of hopping at the outer boundary of the first sub volume correctly. The 3th (rather large) sub volume is necessary, in order to provide correct (isotropic) energy distribution of energies of any state inside the 1st and 2nd sub-volumes.

One can calculate the energy of a carrier, which is initially located in a center of a volume (at the “initial” site), as a sum of charge-dipole interaction energies,

$$E_{\text{central}} = \frac{e}{\kappa} \sum_m \frac{\left(\vec{r}_m, \vec{p}_m \right)}{r_m^3} = E_0 \sum_{i,j,k} \frac{i \sin \theta^{ijk} \cos \varphi^{ijk} + j \sin \theta^{ijk} \sin \varphi^{ijk} + k \cos \theta^{ijk}}{(i^2 + j^2 + k^2)} \quad (1)$$



$$E_0 = \frac{ep}{\kappa a_0^2}, \kappa = 4\pi\epsilon_0\epsilon, \quad (2)$$

p - the dipole moment, ϵ – dielectric constant of the medium; i, j, k - the specified coordinates of the cubic lattice sites (arbitrary integers) and a_0 – the cubic lattice constant (distance between the nearest lattice points), θ, φ – angles that define the spatial orientation of the dipoles at lattice sites. Dipole orientation in space is defined by the random distribution in space (see Figure. 1a).

In analogy, one can calculate energy of a carrier in any site of the first and second sub volumes. Miller–Abrahams hopping rates from site i to site j are presumed [3]:

$$\omega_{i \rightarrow j} = \omega_0 \exp \left(-2\gamma r_{ij} - \frac{E_j - E_i + |E_j - E_i|}{2kT} \right), \quad (3)$$

where ω_0 is the attempt-to-escape frequency, $1/\gamma$ is the decay length of the localized wave function, E_i is the energy of the carrier at the site i , r_{ij} is the distance between sites i and j . The values $T = 295$ K, $2\gamma a_0 = 10$ and $\epsilon = 3$ are used in calculations. Sizes of the sub volumes are the following: $5a_0, 8a_0$ and $15a_0$ (by “size” we mean a half of square side of the volume). If the electron appears in the nearest position of the second sub-volume, event is over. The value $15a_0$ seems to be minimal sufficient to provide size-independence of node energies inside the 1st and 2nd sub volumes with appropriate accuracy.

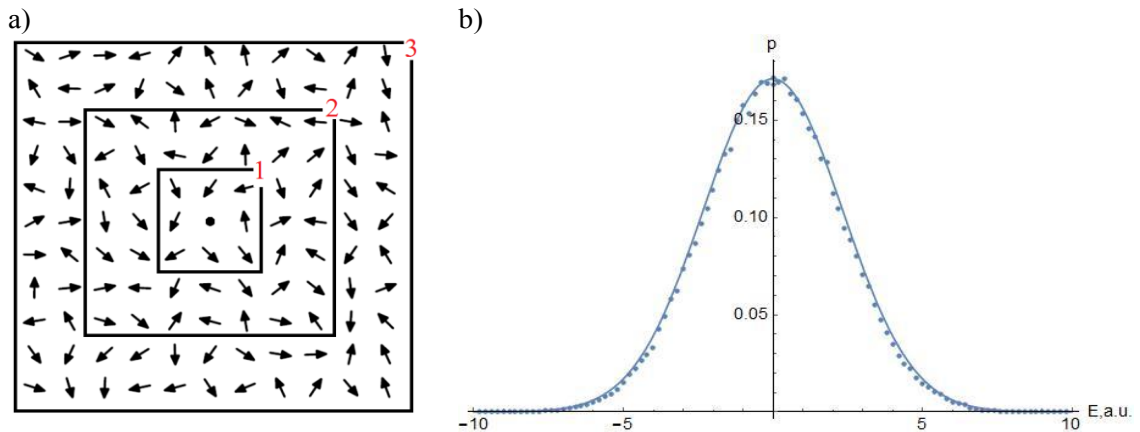


Figure 1. a) Randomly orientated dipoles in the volume and, as the result, b) Gaussian distribution for the energy of the central node.

In order to fix the energy of the central node, $E_{central}$, we choose the interval from $E_{central} - kT/2$ to $E_{central} + kT/2$. If the energy $E_{central}$ is beyond this interval, the procedure of random dipoles setting starts again, until the energy $E_{central}$ falls into the given interval.

To make sure that the energy of the central node has Gaussian distribution, we plot the distribution of energies of the central node for more than 100 000 events (Figure. 1b, E is given in arbitrary units). It is shown that the distribution is well fitted by Gaussian function, and it's mean-square variation corresponds to well-known expression [2]:

$$\sigma = E_0 \sqrt{\frac{1}{3} \sum_{i,j,k} (i^2 + j^2 + k^2)^{-4}} \approx 2.35 E_0. \quad (4)$$

The correlated character of site energies is demonstrated in Figure. 2, where typical distributions of energies of nearest neighbors of an initial (central) nodes are shown for several events. Points with coordinates (r, E) are shown, where r is the distance from the central node to the current node, and E is the energy of the current node. As one can see, there are only several states that are deeper than the central one.

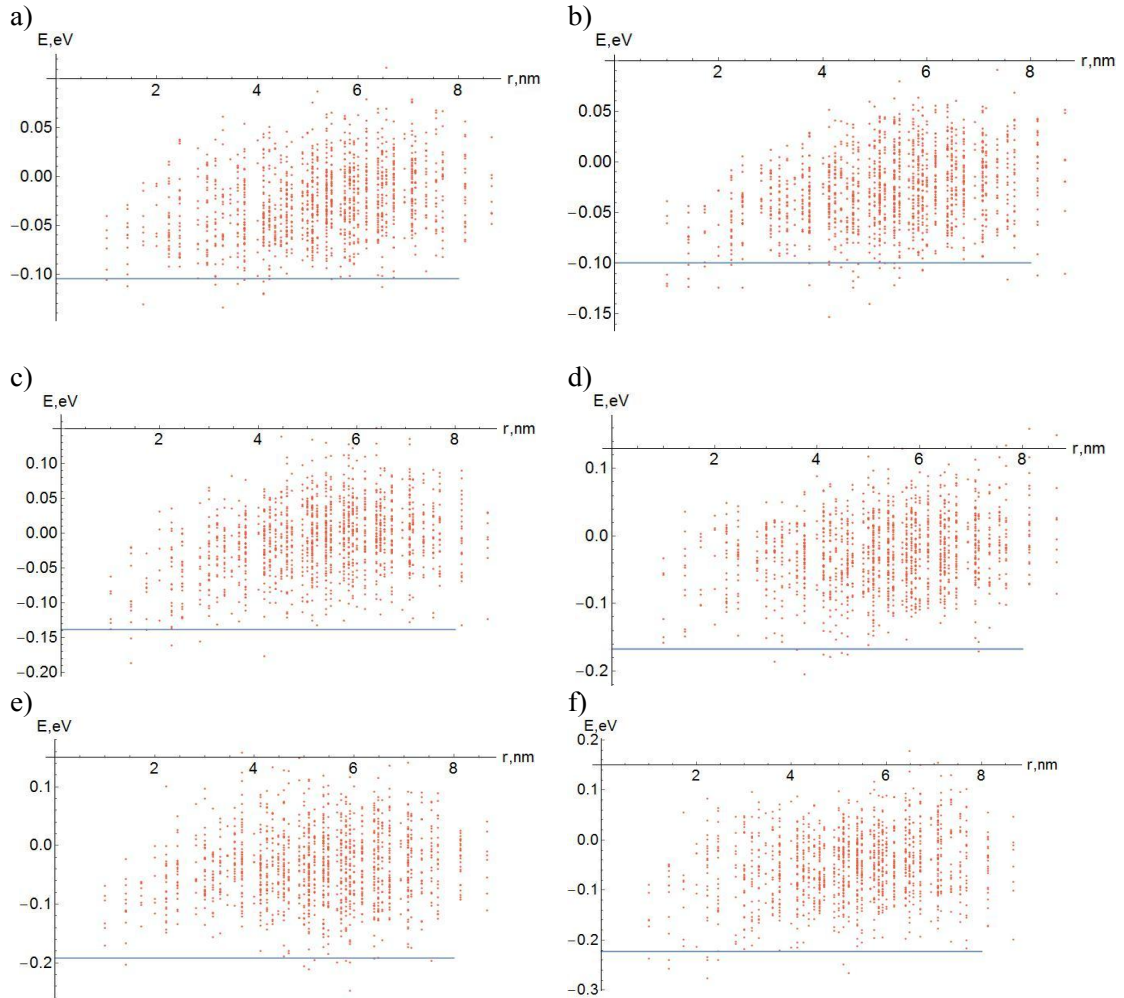


Figure 2. 2D distribution of a node energy versus distance between this node and the central node that shows correlated nature of disorder of the considered system. Parameters are: $E_0 = \sqrt{2}\sigma = 0.05$ eV, $E_0/kT = 2$, $E_{central} = -2E_0$ (a), $-2.2E_0$ (b); $E_0/kT = 3$, $E_{central} = -2E_0$ (c), $-2.2E_0$ (d); $E_0/kT = 4$, $E_{central} = -2E_0$ (e), $-2.2E_0$ (f). The solid line is the energy of the central node calculated according to current dipole orientation.

3. Results and Discussion

The following dependence of mean release time of a carrier from a rather deep initial state on the energy of this state, E_i , should be valid, if transport level concept is applicable:

$$\langle t_{esc} \rangle (E_i) = t_0 \exp[(E_{tr} - E_i)/kT], \quad (5)$$

where $t_0 = \omega_0^{-1} \exp(2\gamma a_0)$ and the effective transport level E_{tr} are constants [1].

Figure. 3 shows the results for mean escape time vs initial energy that were obtained earlier in [1] for the case of non-correlated disorder, plus brand new results for correlated energetic disorder in dipole glass model at various values of the disorder parameter, σ/kT . One has to conclude that new data are in very proximity with the results that were obtained for non-correlated disorder. However, it is clear, that stars, representing the result for correlated disorder, are located a little bit higher than the results of [1]. So there is the difference, but transport levels for both cases are close enough to each other (within the interval kT).

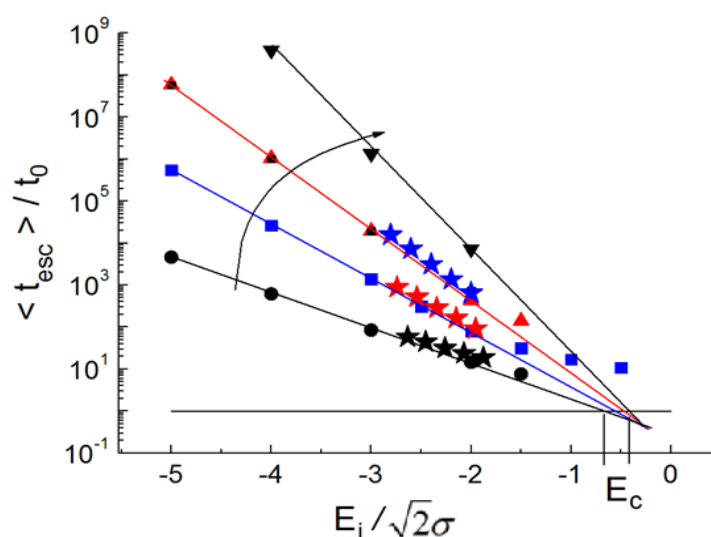


Figure 3. Mean escape time vs initial energy, parametric in disorder parameter, σ/kT : 1.414, 2.12, 2.83, 4.0 (it increases as shown by arrow), $T = 295K$, providing uncorrelated disorder [1]. Stars are brand new results for correlated disorder for $\sigma/kT = 1.414, 2.12, 2.83$. Time and initial energy are normalized by the values $t_0 = \omega_0^{-1} \exp(2\gamma a)$, and $\sqrt{2}\sigma$, respectively. Horizontal line shows the level $\langle t_{\text{esc}} \rangle = t_0$, and vertical dashed lines shows the values of E_c .

4. Conclusion

Following the work [3], one can conclude, that the concept of effective transport level is applicable to the organic materials with correlated disorder. Moreover, both the absolute values and dependence of this energy level on the disorder parameter, σ/kT , is very similar to the same in the case of uncorrelated disorder [1].

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