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Model of Charge Carriers Thermalization in Organic Semiconductors

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The study of the process of electric charge carrier thermalization in molecular semiconductors is presented. For the strong interaction of the photogeneration center with its neighbors the direction of the initial velocity of the charge carrier is independent on the incident light parameters. In the case of weak interaction the initial velocity of the charge carrier is almost perpendicular to the direction of light propagation. The thermalization process is described by Langivin equations. The strength of the photogeneration center interaction with neighbors determines the thermalization length dependence on the ambient temperature and the frequency of the incident light beam. Comparisons with experimental results are presented.

Keywords: Electric; charge; carrier; thermalization; photogeneration; Langivin equations

The process of the electric charge carriers photogeneration in molecular semiconductors has been investigated [1,2] and it was found that this process was multi - stage. Two principal stages can be described. The first is the creation of the geminate electron-hole pairs bound by Cou-

lomb field under the influence of the light quantum. The duration of this stage depends on the electron transition rate and usually lies in the range of (10^{-12} -10^{-10}) s. During this time the neutral exiton states are formed and due to the autoionization turn into the pair ion - «hot» (nonequilibrium) charge carrier, that gives away its surplus energy in the process of inelastic collisions with other atoms and moves to the thermalization length r_T for the thermalization time t_T. The thermalization process is said to be completed when the surplus energy of nonequilibrium charge carrier has decreased to the magnitude ΔW when the carrier's collision with its neighbors becomes elastic. The experimental investigation of the thermalization process [1,2] has shown that the thermalization length depends on the incident light frequency (ν), electric field strength (E) and molecular semiconductor temperature (T). The typical dependence are shown on Fig.1. The set of the models have been proposed [1-2] for the theoretical description of the thermalization process. The common shortcoming of these models is the necessity to make the additional assumptions about the behaviour of the model parameters in order to explain the experimental results. The variety of the approaches is caused by the lack of information on the processes determining the formation and kinetics of exciton state. In particular, the direction of the nonequilibrium charge carrier emission relative to the light quantum momentum has not been not clearly determined. If no significant change of its momentum during the lifetime of an exciton state occurs due to interactions with surroundings, the charge carriers will be emitted perpendicularly to the direction of the incident light quantum. Otherwise the charge carrier velocity direction is not correlated with the direction of the momentum of light quantum. The suggested model allows to answer this question using experimentally obtained dependence $r_T(E)$.The model of the nonequilibrium charge carriers thermalization is based on the following assumptions: 1) the center of photoluminescence are mutually independent; 2) nonequilibrium charge carrier can be considered as a particle being in thermal equilib-

rium with its surrounding; 3) the motion of the nonequilibrium charge carrier is determined by the external electric field, the velocity of the nonequilibrium electric charge produced in the decay of exciton state and the nonequilibrium charge carrier interaction with the medium. Coulomb interaction of geminal couple produced in the decay of exciton state can be neglected. It is most significant when the distance between the geminal charges is small, i.e. when the velocity of nonequilibrium charge carrier is large. It is assumed that interaction with the medium and inertia dominate for large nonequilibrium charge carrier velocities. Taking into account the above assumptions and choosing OX axis along E the following equations can be obtained:

$$\frac{dVi(t)}{dt} + \gamma V_i(t) = \frac{F_L^i(t)}{m} + \frac{eE}{m}\delta_{i,x}, \tag{1}$$

where V_i (i=x,y,z) is the component of the nonequilibrium charge carrier velocity, γ - the friction coefficient, m and e – the mass and the charge of the charge carrier, F_L^i is the Langivin force component, which can be assumed to be δ-correlated:

$$< F_L^i(t) >= 0$$

$$< F_L^i(L_1)\, F_L^i(t_2) >= D\delta(t_1 - t_2)\delta_{ij}, \tag{2}$$

where D is the intensity of Langivin source (here <> denotes ensemble averaging). Initial conditions are:

$$V_i(t)\big|_{t=0} = V_i(0); \qquad V_i^2(0) = \frac{2}{m}(h\nu - A), \tag{3}$$

where A is the energy needed to create an exciton state, h is the Planck constant. The solution of this problem is:

$$< r_T^2 >= \left(\frac{eE}{m\gamma}\right)^2 t_T^2 + \frac{2eE}{m\gamma^2}\left(V_x(0) - \frac{eE}{m\gamma}\right) t_T \left(1 - e^{-\gamma_T}\right) + \frac{1}{\gamma^2}\left(V_x(0) - \frac{eE}{m\gamma}\right)^2 \left(1 - e^{-\gamma_T}\right)^2 + \frac{3K_1T}{m}\left(\frac{2t_T}{\gamma} - \frac{2}{\gamma^2} + \frac{2}{\gamma^2}e^{-\gamma_T}\right) \quad (4)$$

The expressions (4) may be considered in two cases:

$$V_i(0)\sqrt{\frac{m}{h\nu - A}} << 1, \quad (5)$$

$$V_i(0)\sqrt{\frac{m}{h\nu - A}} \approx 1. \quad (6)$$

Condition (5) corresponds to $\Delta p/p << 1$, while (6) corresponds to the violation of this, $\Delta p = p - p_c$; $p(D_c)$- the impulse of the photon (noneqvilibrium charge carrier), it can be shown that for (5):

$$< r_i^2 >\cong \frac{e^2E^2}{4m^2\gamma^4}\left[\ln\frac{h\nu - A}{\Delta W} + \frac{e^2E^2}{2m\Delta W\gamma^2} - \frac{3K_BT}{2(h\nu - A)}\right] + \frac{3K_BT}{m\gamma^2}\left[\ln\frac{h\nu - A}{\Delta W} + \frac{e^2E^2}{2m\Delta W\gamma^2} - \frac{3K_BT}{2(h\nu - A)}\right] \quad (7)$$

In the case (6) one has:

$$< r_T^2 >\cong \frac{2}{m\gamma^2}(h\gamma - A) + \frac{6K_BT}{m\gamma^2} \cdot \frac{\ln^2\left[\frac{eE}{m\gamma}\sqrt{\frac{2}{m}(h\nu - A)}\right]}{\frac{2W_0}{m} - \left(\frac{eE}{m\gamma}\right)^2} \quad (8)$$

Conditions $\frac{eEr_T}{h\nu - A} << 1$ and $\frac{K_BT}{h\nu - A} << 1$ are used in the derivation of (5) through.

Results (7),(8) Obtained with the theoretical model and corresponding experimental data for polyvincarbazole (PVC) [3] are presented in Figure1. Similar experimental dependencies have been oslo reported for other materials [4].

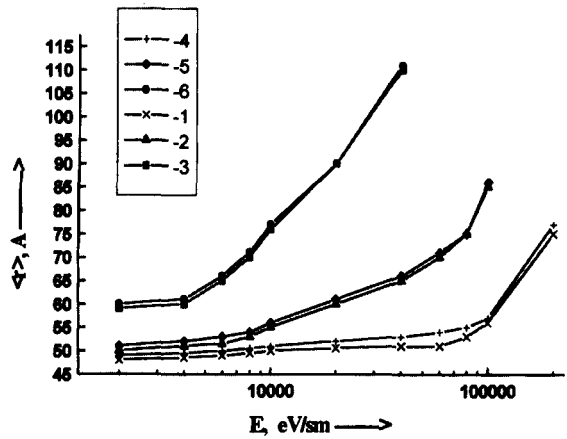

FIGURE 1. The experimental dependence of $r_T(E) = \sqrt{< r_T^2(E) >}$ by light frequency. hν=2,5 eV (1), 2,6 eV (2), 2,8 eV (3). The (4), (5), (6) is the theoretical dependence (with (7))

It is clear that the results of experiments with pentacere and agree with (7). This points to the realization of the condition $\Delta p/p \ll 1$ by thermalization of electric charge carriers in. The results of experiments with PCV on the other hand obey expression (8). This is possible when $\Delta p/p \sim 1$, in the case of large change of momentum of exciton state during its lifetime.

A model of the electric charge carriers thermalization of is proposed to explain the thermalization process during the decay in the external electric field of an exciton state, produced by light absorbtion in media with low charge mobility level. The model explains without in-

troduction of extra model parameters temperature, field and energy dependence of the thermalization length. Character of the temperature dependence of the thermalization length depends significantly on the interaction of an exciton state with neighbors. In case of weak interaction when momentum exchange between neighbors is insignificant, r_T decreases with the medium temperature linearly or almost linearly. When momentum exchange is strong (i.e. when there is no correlation between the momentum direction in the beginning and in the end of its lifetime) r_T only weakly depends on temperature. The specific shape of the dependence is determined by the details of the excess energy return by nonequilibrium charge carriers to the surroundings. Thermalization length of the photogenerated charge carriers in case of weak interaction of exciton states with neighbors increases faster with the electric field than for strong interaction. Increase in energy of the light quanta, creating the exciton states in molecular semiconductors leads to the increase in the thermalization length. In case of weak interaction this is increase is logarithmic, while for strong interaction it is linear.

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