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ON THE PROCESSES OF THE CHARGE TRANSFER IN THE ELECTRICAL CONDUCTING POLYMER MATERIALS

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Abstract. The analysis of charge transfer processes in the electrical conducting solid polymer systems has been carried out. The processes in these systems are divided to two types. The first type is the process of charge transfer between electrodes and particles while the second one – the process of the charge transfer between conductive particles. The description of medium is carried out using Green temperature functions of polarization operators for the molecular medium. It permits taking into account the effects of frequency and space dispersion. The analytical expressions for kinetic parameters of the charge transfer processes from electrodes to particles and between particles in condensed matter have been obtained. The comparison of the general theoretical dependence of the current in electric conducting polymer composites (ECPC) on the average distance between conducting particles with analogical dependence for some real ECPC are presented in the paper.

Keywords: polymer composite, charge transfer, vector-potential, Hamiltonian, Green function.

1. Introduction

Recently so-called nontraditional electrical conducting materials, particularly composites containing a dielectric basis (ceramics, polymers) and conducting dispersive fillers (carbon-graphite and metallic powders) display a growing competition to traditional conductors (*e.g.* metals or classical semiconductors). Such situation is due to many positive characteristics of these materials, among which are high corrosion stability, accessible technology of production and low cost. Now there are many scientific and technical works both of theoretical and experimental character devoted to the noted materials [1-5].

Growth of ECPC conductivity with the increase of conducting filler content is the rule without exclusions [1-4, 6]. The specific feature of this dependence is an increase of specific volumetric electric conductivity γ or a decrease of it inverse specific volumetric electric resistance r at definite (for a particular composite) threshold filler concentration, induced by an insulator-conductor transition. This transition conforms to the so-called threshold of proceeding, or percolation. In this case γ value jump, which may reach several decimal degrees, is stipulated by formation of a continuous chain of filler particles in the polymer matrix – the infinite cluster [7, 8].

At present the problem of the ECPC conductivity mechanism is still to be discussed. Some investigators [9, 10] claim that the charge transfer is conducted by chains consisting of filler particles having direct electric contact. In the opinion of other authors [11, 12] ECPC conductivity is caused by thermal emission of electrons through spaces between particles. There is another opinion that current exists in ECPC with air gaps of polymer films between filler particles. In this case electrons, which energy is lower than the potential barrier value may be tunneled through it, if their own wave-length is comparable with space width of insulating film [13-15]. The Wessling model [16] considers formation of conductive chains as the process based on the non-equilibrium thermodynamics. At present the percolation theory [17] is widely used for calculations of γ for conducting composites (with both organic and inorganic binders). According to this theory γ of composites consists of non-interacting phases. Experimental and theoretical studies of composite conductivity [18, 19] were conducted in superfine gaps between graphite particles. In this case a significant importance was attached to the polymer molecule state in the gap – the filler particles should have

a hypothetic form of a truncated cone. First of all it is the process of the electron transfer from one electrode to the electric conducting particles distributed in the polymer matrix, while second one – electron transfer from one conducting particle to another in the polymer matrix. The third type of the processes is electron transfer from conducting particle to the second electrode in the polymer. The analysis of works on the investigations of electrically conducting properties of ECPC induces one general conclusion: despite a variety of the above considered models of electrically conducting ECPC, unfortunately none of them could pretend to versatility. Each model includes one or several approximations and suppositions, which aggravate the correctness of estimations of ECPC conducting properties. That is why the comparison of theoretically calculated data with the experimental results usually gives deviations that reach several orders in some cases. The coincidence is rarely reached at definite concentrations of conducting filler and specific conditions of the composite production.

In the presented work a new approach to charge transfer processes in the polymer materials containing the conducting fillers has been proposed.

2. Results and Discussion

2.1. The Hamiltonian System

The processes of charge transport from the electrode to particle may be described analytically at choosing of the concrete system for which it is possible to write the Hamiltonian system. A principal difficulty of investigation of charge transfer processes is connected with the necessity of using of quantum approach. In the frame of the quantum transfer approach there is yet no models generally accepted for the processes of charge transfer in the irregular systems. Using of such apparatus of mathematical physics as the apparatus of Green temperature function (GF) allows describing complex condensed systems and processes of charge transfer in them. This technique allows unification of theoretical approaches, using widely different models for describing of the effects of the system of frequency and space dispersion [20-23].

2.2. Current Density for the Process of Charge Transfer from Metal or Semiconductor Electrode to the Conducting Particles in the Polymer Matrix

The calculation of the current density connected with the process of charge transfer from electrode to

particle may be carried out on the basis of quantum-mechanical calculations for process of transition between two electron states. The density of cathode current may be presented as:

$$i_c = e \frac{N_0}{S} \int d\epsilon r(\epsilon) n_F(\epsilon) n_F(\epsilon_1) W_c(\epsilon, \epsilon_1)$$

where e – the electron charge, S – electrode surface, N_0 – number of particles in the system volume of particles V_0 , $r(\epsilon)$ – density of single electron states in the electrode, $r(\epsilon_1)$ – density of single electron states in the particle, $n_F(\epsilon)$ – Fermi function of the electron distribution, $W_c(\epsilon, \epsilon_1)$ – probability of the electron transfer from given energetic level of the electrode ϵ on the given energetic level of particle ϵ_1 .

The electron transfer may be both electron non-adiabatic and electron adiabatic. Usually in the wide range of the parameters the process of charge transfer of the electron is electron-nonadiabatic transfer and below first of all we will consider electron-nonadiabatic transfer of the electron.

At integration on the energy it must be noted that usually the contribution to the integral on energies possesses small range of energies and formal integration on energies may be carried out in the infinite limits. The probability of the electron-nonadiabatic transfer of the electron is expressed as:

$$W_c(\epsilon, \epsilon_1) = \frac{b}{i} \exp(bF_i) \int dq S_p \left[\exp(-b(1-q)H^i L \exp(-bqH^f)L) \right]$$

Omitting the cumbersome calculations we present the quantum expression for density of cathode current of heterogeneous process with participation of metallic or semiconductor electrode with Fermi distribution:

$$i_c = ep \left| L_{fi}(\mathbf{R}^*, \mathbf{y}^*) \right|^2 \int d\epsilon d\epsilon_1 kT r(\epsilon) r(\epsilon_1) \cdot \exp(-2 \ln(\sin pq^*)) f(\mathbf{R}^*, \mathbf{y}^*) U(\mathbf{R}^*, \mathbf{y}^*) \cdot \exp[-bq^* \epsilon h - bq^* \Delta F - y^m(\mathbf{R}^*, \mathbf{y}^*, q)]$$

$$b = 1/kT$$

where ΔF is free energy of the process. The star in the designation marks means the value of this coordinate in the point of maximum at calculation of corresponding integration by given coordinate, as a rule, by the saddle-point method. The saddle-point θ^* may be found from equation:

$$\epsilon h + b\Delta F + \frac{\partial y^m(\mathbf{R}^*, \mathbf{y}^*, q)}{\partial q} + 2p \operatorname{ctg}(pq) = 0$$

In these formulae L_{fi} is the resonance integral from interaction of particle with surface of semiconductor or metal electrode. Matrix element is calculated by using of wave functions in the frames of concrete model for particle. The resonance integral L_{fi} may be considered as some phenomenological parameter. Arguments of this

resonance integral characterize the geometrical characteristic of process, distance to surface (R), spatial orientation of particle (Ψ) at transfer of charge. Function $U(R^*, y^*)$ is calculated for concrete processes allowing for the geometry of electrode and particles. Function $f(R^*, y^*)$ presents the function of distribution of admixture particles. This function may be model one, connected with particles concentration. Function $y^m(R^*, y^*, q)$ is one of reorganization of the polymer medium. Its formal expression has the view:

$$y^m(R^*, y^*, q) = \frac{1}{p} \int dr dr_1 \Delta E_i(r, R^*, y^*) \Delta E_k(r, R^*, y^*) \cdot \int_{-\infty}^{\infty} dw f(w) \frac{sh \frac{bw(1-q)}{2}}{w^2 sh \frac{bw}{2}} sh \frac{bwq}{2}$$

where ΔE is the change of the electrical field voltage of admixture particle and electrode at process of charge transfer.

This function in general describes both the processes of tunnelling of an electron and classic reorganization of medium at charge transfer.

Let us introduce the energy of reorganization of the polymer medium by means of relation

$$E_r^m(R, y) = -\frac{1}{2} \int dr dr_1 \Delta E_i(r, R, y) g_{ik}^R(r, r_1, w=0) \Delta E_k(r_1, R, y)$$

In the factorization approximation for function g^R over spatial and time coordinates the medium reorganization function may be presented in view:

$$y^m(R^*, y^*, q) = E_r^m \frac{4p}{h} \int_{-\infty}^{\infty} dw f(w) \frac{sh \frac{bw(1-q)}{2}}{w^2 sh \frac{bw}{2}} sh \frac{bwq}{2}$$

At integration over r and r_1 it is necessary to take into account the structure of medium and the situation when both effects of spatial dispersion of medium (function $g(r, r_1)$) and the effects of its frequency dispersion (function $f(\omega)$) will be described by different model functions allowing for existing of definite modes of polymer polarization.

The carried out calculations show that complete fulfilling of the analytical calculations is impossible and it is necessary to carry out the numerical integration.

The activation energy may be defined by formula:

$$E_a = -2 \ln(\sin pq^*) + q^* (1 - q^*) E_r^m - q^* eh - \Delta F q^*$$

The above presented relations are valid also for the processes of the charge transfer of the electron from particle to electrode at corresponding change of marks of energetic parameters.

The calculations of the kinetic parameters for processes of electron-adiabatic processes of electron may

be considered in detail analogically to nonadiabatic processes. However, another method of estimation of the parameters for adiabatic processes may be used.

The probability of transfer may be presented in view:

$$W_{ad} = A_{ad} \exp(-bE_a)$$

In this formula the pre-exponent multiplier may be obtained from analogical expression for nonadiabatic process by substituting of electron resonance integral on the critical value by the formula:

$$L_c = \left(\frac{kTE_r^m w_m^2}{p^3} \right)^{1/4}$$

where critical value for single-frequency model of medium (with frequency ω_m) has the view: $L \rightarrow \frac{L_c}{\sqrt{2}}$

The activation energy of the process is defined by the way in which the adiabatic term is designed from potential energies of the channel terms of initial and final states U_i and U_f .

$$U = 0.5(U_i + U_f) - (0.25(U_i - U_f)^2 + L^2)^{0.5}$$

Further on the points of the minimum and the maximum of the system energy and the activation energy is defined as difference between values corresponding to maximum and minimum at initial state.

2.3. Processes of Charge Transfer between Admixture Particles in the Polymer

The processes of charge transfer in the conducting polymer systems are defined by a number of factors. First of all those are the geometrical parameters of conducting particles, their shape, mutual orientation of interacted particles, possibility of adsorption of polymer molecules on the surface of conducting particles, and effects of "solvation" of conducting particle with polymer molecules. Similar details of such systems are mainly defined by method of preparation of conducting polymer material and properties of components. Depending on peculiarities of structure of composite material it is necessary to use one or another model for calculation of kinetic parameters. So, if the polymer molecule is chemically adsorbed on the surface of conducting particle actually instead of the charge transfer process between metal particles in the polymer matrix it is necessary to consider the process with participation of adsorbed particles. So, the adsorbed particle becomes the essential element of the process. In all kinetic parameters intramolecular reorganization of adsorbed particles will be presented. All calculations will be essentially complicated, but their execution in sufficiently correct form is possible.

One of the serious problems at investigation of such systems is distribution of electromagnetic field near particle surfaces. This distribution often plays the defining role at calculation of kinetic parameters. The picture of distribution of the field essentially depends on “solvating” capability of the polymer molecules. For solvated particles it is also necessary to use the model of particles with oscillation subsystem in which only in some cases it is possible to describe which exactly chemical bonds participate in the oscillation, however some generalized oscillated modes can be foreseen. There is a possibility of analytical calculations, although in this case the definite number of parameters are arisen, which are the characteristics of the system, and whose numerical estimation are very approximate.

The process of charge transfer between admixture particles in the polymer is considered as process of transfer between two metal electrodes in the condensed medium. The model for such processes may be presented on the basis of the above conducted calculations for processes of transfer between electrodes and particles. For conducting such calculations it is necessary to detail the Hamiltonian system. It may be used the same model approximations for describing of particles (1 and 2) and medium, which were used in the last section. In the result for initial state the Hamiltonian one gets the view:

$$H^i = H_{p1}^i + H_m^i + H_{p2}^i + H_{p1,m}^{int} + H_{p2,m}^{int} + H_{p1,p2}^{int}$$

Analogical view has the Hamiltonian of the final state.

2.4. The Rate Factor of Charge Transfer Process between Conducting Particles

The current density for the process of electron transfer from particle 1 to particle 2 in the polymer matrix has a view:

$$i_c = ep \left| V_{fi}(\mathbf{R}^*, \mathbf{y}^*) \right|^2 \int d\mathbf{e} d\mathbf{e}_1 k T r(\mathbf{e}) r(\mathbf{e}_1) \cdot \exp(-2 \ln(\sin pq^*)) f(\mathbf{R}^*, \mathbf{y}^*) A(\mathbf{R}^*, \mathbf{y}^*) \cdot \exp[-bq^* e h_{12} - bq^* \Delta F_{12} - y_{12}^m(\mathbf{R}^*, \mathbf{y}^*, q)]$$

Here the critical point for q^* is defined from equation:

$$e h_{12} + b \Delta F_{12} + \frac{\partial y_{12}^m(\mathbf{R}^*, \mathbf{y}^*, q)}{\partial q} + 2pctg(pq) = 0$$

The preexponent multiplier is calculated for concrete particles allowing for the particles geometry, space orientation and the distance of electron transfer.

For activation energy of transfer process we have:

$$E_a = -2 \ln(\sin pq^*) + q^*(1 - q^*) E_r - q^* e h_{12} - \Delta F_{12} q^*$$

The presented expressions allow one to conduct simple estimations of process kinetic parameters in frames of strongly simplified models. In this way one could

calculate the electron kinetic parameters using average magnitudes of admixture concentrations and, consequently, to get average magnitudes of parameters.

At estimation of kinetic parameters it must be foreseen that direct charge transfer takes place really in the limits of 30 Å, and that because of electron tunnelling. The charge transfer through intermediate state, naturally, is possible, but the probability of the final process will be equal to the product of probabilities of all elementary acts of electron transfer.

2.5. Scheme for Carrying out of Quantitative Estimation for the Processes

The schemes of calculations for estimation of kinetic parameter values of different processes are presented below:

1. For calculation of the kinetic parameters first of all it is necessary to define what particles react and what the reaction medium is as well as what electrodes are used at real measurements. It is necessary also to have maximal information about electrode, its zone structure, bending of zones near the surface, etc.

2. Introduce the degrees of freedom of the reaction and divide them on classic and quantum for medium. Classical degrees of freedom may be the ones satisfying the condition:

$$th \left(\frac{w_i(1-q^*)}{2kT} \right) \approx \frac{w_i(1-q^*)}{2kT} \ll 1 \quad th \left(\frac{w_f q^*}{2kT} \right) \approx \frac{w_f q^*}{2kT} \ll 1$$

At fulfilling of preliminary calculations the number 0.5 may be taken as value of θ^* .

3. Fulfill the estimation of the medium reorganization energy by simple formulas [23]. However, it is necessary to take into account here, that in the dependence of medium only definite modes of polarization are reorganized and, consequently, instead of static dielectric penetration the values of the dielectric permittivity from left and right sides of corresponding pick of absorption must be used. After preliminary estimation for final calculations a model for describing of spatial dispersion of medium must be selected.

4. Define or estimate the electron resonance integral or dipole moment of transition using quantum-chemical methods, sums law, and fulfilled calculations for similar systems. It must be foreseen that quantum-chemical calculations allow one to conduct calculations either in vacuum or in medium with static-dielectric background, but not in medium with complex structure. Therefore, at final calculations of the kinetic parameters of processes it is often necessary to introduce the corresponding corrections in the results, e.g. in the characteristic value of decay of the resonance integral.

5. Define the character of charge transfer process, whether it is electron-nonadiabatic or adiabatic. For electron-nonadiabatic process the above given methods must be used and for the adiabatic ones – the transfer rule, in which is the method of calculation of pre-exponent, rate factor and definition of activation energy of the process after calculation of transition configuration and the finding of the coordinates of minimum of initial system state and maximum in the transition state. The calculation of the Landau-Zener parameter may be carried out by using of formula:

$$g_e = \frac{2pL^2}{|u||\Delta U|}$$

where u is the rate of movement over the reaction coordinate of the system near transition configuration, ΔU is the difference of inclinations of terms of potential energy near point of their crossing.

If the condition $g_e \gg 1$ is fulfilled then the process has an electron-adiabatic character. At calculation of the kinetic parameters [23] the adiabatic terms must be used. The transmission factor in this case is $\kappa \approx 1$. At fulfilling of reciprocal condition the process has electron-nonadiabatic character.

6. Define transition configuration. The definition of transition configuration over spatial and rotational coordinates of reaction is more complex task as there are no general methods for that. It is necessary to have information about distribution of the reacting particles in the medium to use the right function for their distribution. The information about possible mutual orientation of reacted particle is necessary. At writing of the potentials of reagent interactions all this information is necessary for introduction of reaction coordinates and calculation of transition configuration by them.

7. Calculate the transition coefficient for heterogeneous reaction θ^* .

8. Estimate the activation energy for classic degree of freedoms and tunnelling factor – for the quantum ones.

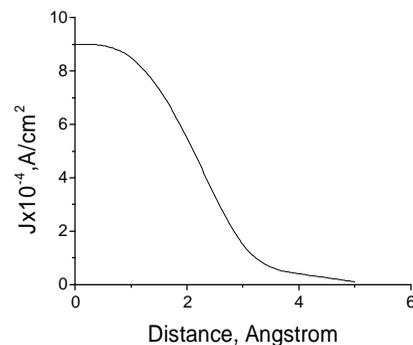
9. After conducting of preliminary calculations make the models of processes for each stage of electron transfer process more exact, co-ordinate the models of separate stages and conduct the exact calculations on the full scheme for all systems.

As was noted above, experimental data treatment requires exacting of parameters entered to the results of analytical calculations obtained in the frames of theoretical models. However, some conclusions may be made on the basis of semi-classical estimations of the parameters. We will provide estimations for metallic electrode and electrical conducting particles.

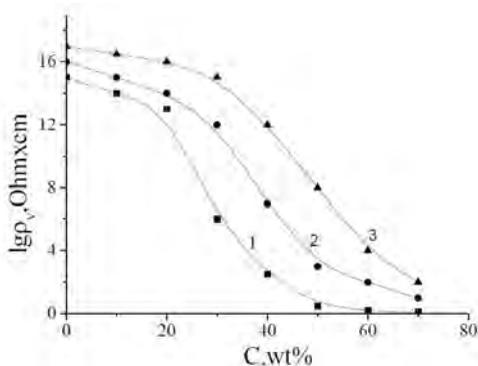
One of the defining factors at calculation of the process rate constant is the distance of transition. At the same time this parameter defines often the character of process, whether it is

adiabatic or non-adiabatic. It may be shown qualitatively that if the character of the charge transfer process is adiabatic the rate constant weakly depends on transfer distance because the main dependence in the process rate constant on the distance is presented through electron resonance integral. At the same time, for adiabatic processes it is necessary to change the electron resonance integral to its critical value, which is not presented by the function of the transfer distance. The calculations in different systems show that in the condensed medium the electron transfer process has adiabatic character only on rather small distances. Consequently, on small distances the rate constant of the process will not be dependent on distance. Moreover, the value of rate constant will mainly be dependent on the medium properties and for very rough model of homogeneous, isotropic local medium in the frames of single mode model it will be presented by frequency of this mode ω_m and by energy of the reorganization of medium E_r^m , in these case the square of the electron resonance integral must be changed to the following value:

$$\frac{(kTE_r^m)^{1/2}}{2p^{3/2}} w_m$$



a)



b)

Fig. 1. Dependence of current density on the distance between conducting particles in the ECPM calculated theoretically (a) and experimental data of the specific volumetric electric resistance dependence on the conducting filler concentration in ECPM for different composites (b): ECPM based on polydimethylvinilsiloxan with silver nanoparticles of 50–100 nm (1); ECPM based on epoxy resin with nickel nanoparticles of 200–250 nm (2) and ECPM based on polytetrafluoroethylene with graphite nanoparticles of 200–300 nm (3)

In the last expression the energy of medium reorganization depends on the electron transfer distance, but this dependence has relatively weak character. At variation of distance of transfer by 60–70 % the reorganization energy is changed by about 25–40 %, depending on the model.

The electron resonance integral for adiabatic processes of the electron transfer is exponentially decreasing function of the distance.

$$L(R) = L_0 \exp\left(-\frac{R}{\Delta}\right)$$

For many processes of nonadiabatic electron transfer the characteristic distance of the decay of electron resonance electron Δ (it is proposed that the distance R is measured in angstroms).

Qualitatively the current density in the polymer system with electrical conducting filler is the function of distance between conducting particles and graphically corresponding dependence has the graphical view presented in Fig. 1 ($\Delta = 0.4 \text{ \AA}$).

For comparison of the theoretically calculated dependences of electrical current density on the average distance between conducting particles in the polymer matrix with experimentally obtained results for three polymer composites, containing silver, nickel and graphite nano-powders the curves are presented in Fig. 1, although they are distinguished one from another by coordinates titles. However it is easy to understand that they have equivalence character – increasing of the average distance between conducting particles is equivalence to decreasing of the filler concentration and electric current is inversely proportional to the electric resistance of these materials. The curves in Figs. 1a and 1b show the symbatness between theoretical and experimental curves. Therefore theoretical approach to describing of the nature of charge transfer in the polymer composites, containing the conducting filler, principally may be used as the basis of the main processes of charge transfer happening in these heterogeneous systems.

3. Conclusions

Comparison of theoretically calculated values of the density of electrical current depending on the average distance between conducting particles shows that the considered approach to the analysis of processes of the charge transfer in electrical conducting polymer composites satisfactorily describes the conducting properties of these materials.

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ПРО ПРОЦЕСИ ПЕРЕНЕСЕННЯ ЗАРЯДІВ В ЕЛЕКТРОПРОВІДНИХ ПОЛІМЕРНИХ МАТЕРІАЛАХ

Анотація. Проведений аналіз процесів перенесення зарядів в твердих електропровідних полімерних системах. Процеси розділено на два типи: перший тип відноситься до процесу перенесення заряду від електродів на струмопровідні частинки, а другий – між цими частинками. Середовище описано за допомогою поляризаційних операторів функції Гріна для молекулярного середовища, що дає можливість враховувати частотні ефекти і просторову дисперсію. Одержано аналітичні вирази для кінетичних параметрів перенесення заряду від електродів на частинки і між частинками. Проведено порівняння результатів, отриманих теоретичними розрахунками залежності електроструму від середньої відстані між провідними частинками електропровідного полімерного композиту (ЕППК) з аналогічною залежністю, отриманою для реальних ЕППК.

Ключові слова: полімерний композит, перенесення заряду, вектор потенціалу, Гамільтоніан, функція Гріна.