UDC 538.9

INVESTIGATION OF BIMOLECULAR INTERACTIONS WITH THE USAGE OF COMPUTER MODELING

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The results of computer modeling of bimolecular interactions in matrices with different initial order of reagents are presented. Change in distributions of reagents on the induced surface is considered by results of the multifractal analysis. Obtained results allowed to establish that slower kinetics of decrease in matrices with greater extent of order is observed, for which different kinetic regimes are observed in different points of time.

Keywords: cellular automata, multifractal analysis, heteroannihilation interactions.

INTRODUCTION

The practical application of hetetogeneous molecular structures in the fields of quantum electronics and applied optics determines interest to the methods of their receiving and studying their properties. Such kind of structures with adjusted dimensions aren't created by straight technical methods, but they are spontaneous formed at the determine macroscopic conditions [1]. This fact makes us to consider nonclassical laws of decrease of interacting particles [2]. In this case, kinetic dependences contain information about change of the type of reagents distribution and about efficiency of energy transfer processes carrying out simultaneously in different local areas with various values of order degree. As a result of that fact change of energy transfer efficiency of electron excitation in these systems is determined by the change of fractal dimension of reagent distribution.

COMPUTER MODELING

To describe kinetic laws of behaviour of such systems in this work there is given the computer modeling method of energy transfer processes of electron excitation. Interaction occurs between donor molecules fixed by physical sorption and energy acceptor molecules, mobility of which is determined by sorption properties of the surface and temperature of the matrix.

Offered model bases on the usage of the probabilistic cellular automata. Modeling of paired heteroannihilation interactions is carried out over discontinuous time spans, assigned by number of iteration N, at the temperature of matrix 273K. The ratio of concentrations of interacting molecules was selected equal to 1:1. Initial distribution of particles on the surface changed from accidental to clustered by the special way of each sorts on knots of lattice with different order. Probability of interaction p is selected in the range from 0.2 to 1. Significance $p=1$ corresponds to momentary interaction of selected donor particle with any of acceptor particles, found on one internodal distance (sphere quenching radius), in other words passing corresponds to diffusion-controlled reactions. Significances of probabilities of interaction $p<1$ correspond to passing of kinetical-controlled reactions. The analysis of influence of reagents initial order on kinetics of paired interactions is conducted at two significances extent of covering by donor molecules at initial point of time: σ=0.4% and σ=0.2%. The character of distribution of interacting particles on the surface at different time regions of kinetic dependences is determined by the kind of distribution function of particles on cells of adjusted dimension and analyzed in correspond with result of mutifractal analysis (MFA). It allows determining such parameters of system as integrated fractal dimensions,

order and homogeneity parameters, entropy. When MFA is conducted dimension of cell is determined by number of knots of lattice.

RESULTS AND DISCUSSION

The results of conducted modeling allow revealing some correlations between fractal and thermodynamical parameters of system at adjusted extent of covering surface by one sort of particles (Tab I).

Table I-The Significances of Initial Order of Reagents Δ, Integrated Fractal Dimensions D_q, Entropy S of Simulated Matrix at Different Significances of Extent of Surface Covering by the Donor Molecules:

Table I.

σ=0.4% $p = 0.7$				
Δ	D_0	D_1	D_2	S
0.247	1.996	1.963	1.937	6.251
0.249	2	1.975	1.955	6.316
0.236	1.999	1.971	1.932	6.278
0.259	1.997	1.963	1.935	6.258
0.351	1.998	1.951	1.913	6.211
σ=0.2% $p = 0.7$				
Δ	D_0	D_1	D_2	S
0.371	1.978	1.931	1.892	6.116
0.301	1.988	1.947	1.911	6.154
0.350	1.976	1.927	1.888	6.094
0.367	1.978	1.917	1.868	6.049
0.513	1.954	1.875	1.799	5.855

Independently from extent of covering surface by interacting particles, the increase of initial order in distribution of reagents leads to decrease of integrated fractal dimensions D_q and informational entropy S of system. That fact determines thermodynamical conditions of molecular clusters formation on the surface. Smaller significances of S and D_q correspond to more balanced conditions of surface structures formation and higher level of self-organization of system as a whole.

Influence of thermodynamical and fractal parameters of system on the kinetics of heteroannihilation interactions is presented in Fig. 1.

The analysis of kinetic dependences reveals that independently from extent of covering surface σ the increase of initial order parameter reduces to deceleration of interaction kinetics. This evidently associated with local clusters formation on the surface with high density of donor molecules and leads to increase of time of reagents contiguity.

The process of annihilation of interacting pairs accompanies with decrease of system entropy. The faster change of entropy is observed when interactions between nonclustered particles predominate. As reagents divise and molecular clusters are formed on the surface the rate of entropy change increases (Fig. 2).

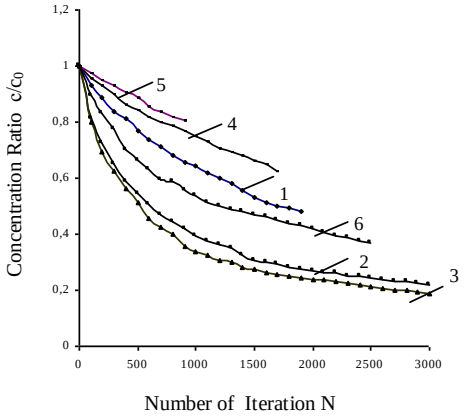

Fig.1. Influence of probability of interaction and extent of covering surface on kinetics decrease of donor molecules distributed on the surface with adjusted order (Δ=0.3±0.005; c- donor molecules concentration at set point of time, c0-initial donors concentration: 1) σ=0.4%, p=0.2; 2) σ=0.4%, p=0.5; 3) σ=0.4%, p=1; 4) σ=0.2%, p=0.2; 5) σ=0.2%, p=0.5; 6) σ=0.2%, p=1.

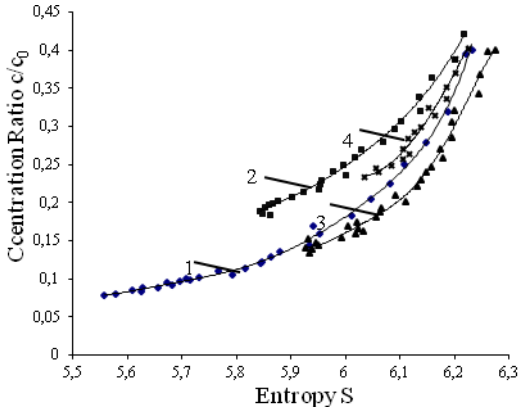

Fig. 2. Change of system entropy at heteroannihilation interactions:
1) p=1, Δ=0.292; 2) p=1, Δ=0.371; 3) p=0.2, Δ=0.273; 4) p=0.2, Δ=0.363.

As evident from Fig. 3 at constant extent of covering in more ordered systems we could observe denser distribution of particles at cells and simultaneous increase number of vacant cells, that correspond to space division parts of surface with higher local density of particles. Decrease of extent of covering surface in process of bimolecular interactions at constant local order of reagents takes place in the result of fast destruction single molecules as compared with the molecules lying in cells with more local density.

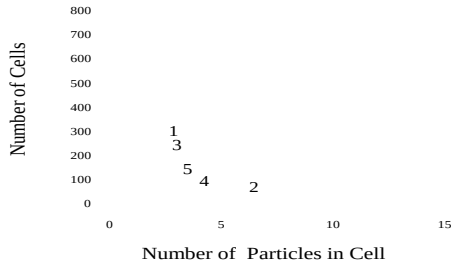

Fig. 3- Dependence donor molecules distribution function on the surface on extent of covering surface σ and initial order Δ: 1) σ=0.4%, Δ=0.272; 2) σ=0.4%, Δ=0.351; 3) σ=0.2%, Δ=0.273; 4) σ=0.2%, Δ=0.521; 5) σ=0.2%, Δ=0.350.

CONCLUSION

Thus, obtained researches showed that in molecular systems the kinetics of heteromolecular interactions appreciably depends on the extent initial order of reagents, probability of interaction and of the extent of surface cover by reagents. In more ordered matrixes heteromolecular interactions proceed mainly between clustered particles whereas interactions between nonclustered molecules of reagents predominate in systems with accidental distribution of particles.

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Article accepted for publication 24.05.2013