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COMPUTER MODEL OF SELF-ORGANIZATION OF CLUSTER SYSTEMS IN SOLIDS

A computer model of cluster formation is proposed and the dependence of the cluster system parameters on the initial modeling conditions is obtained.

The study of cluster formation in solids is associated with the complexity and laboriousness of experiments. The main problems are related to the fact that to obtain reliable information about the structure and properties it is necessary to synthesize clusters with a wide range of parameters and create a reliable system for their diagnostics. In this regard, it makes sense to use simulation and statistical modeling, and the most reliable predictions of the properties of such systems are computer calculations, conducted, in particular, by the Monte Carlo method.

To solve the problems associated with the practical study of cluster systems, a software complex for clustering modeling (SCCM) has been developed, in which the cluster-cluster and cluster-particle interactions are simulated, and this system is typical for the structure of various formations in solids – set of particles, cracks, structural heterogeneities, voids, pores, interfaces, etc.

The following tasks have been accomplished in the development of SCCM:

- a method for generating a cluster system was conducted;
- a method of multiple marking of Hoshen-Kopelman clusters for finding the percolation threshold on a square, cubic and multidimensional lattices was implemented;
- worked out: algorithms for clusters numbering, clusters distribution by size, calculating a number of characteristics, such as radius of gyration, anisotropy level; the determination of critical indicators, such as the correlation length index, the cluster power growth index, and the dimensions of (fractal, correlation) percolation cluster and clusters whose mass exceeds 20% of its mass;
- it is provided for obtaining results of analysis of the properties of the cluster system in a variety of modeling cycles to obtain a graphical and textual representation of the data.

SCCM is created on a high-level Java programming language using the Oxygen.2 integrated development environment (Eclipse IDE for Java Developers). To determine the place of origin of the transformed section, the Monte Carlo method and the random number generator are used. A multidimensional percolation problem is solved in the model. Simulation of clustering processes is carried out on a field filled with non-zero elements with a certain probability. As the number increases, the particles coagulate and form clusters.

The path of successively increasing a given number of particles is used as an algorithm for the growth of clusters. One of the important things in this process is a reliable random number generator with an uniform distribution: first with its help the coordinates of the clustering centers are selected, and then one of the centers in which the filling process will take place, after which the generator indicates the place where the next part of the growing cluster will be located. The controlling parameters of the computer model of cluster formation are the relationship between the particle size and the field side, the number of acts of attraction of particles at each generation stage, the minimum interaction distance of particles, the length of the percolation cluster connectivity, the choice of the particles interaction law – $1/R^2$ or $1/R$. In addition, in each model experiment, the number of measurements of space on the field, the size of the field, and the number of clustering centers are specified.

When modeling in SCCM, the process of combining particles into clusters is visualized and animated in real time. In the main SCCM window, the 3D visual model rotates in all directions and the simulation field is scaled, as accordingly the entire cluster system.

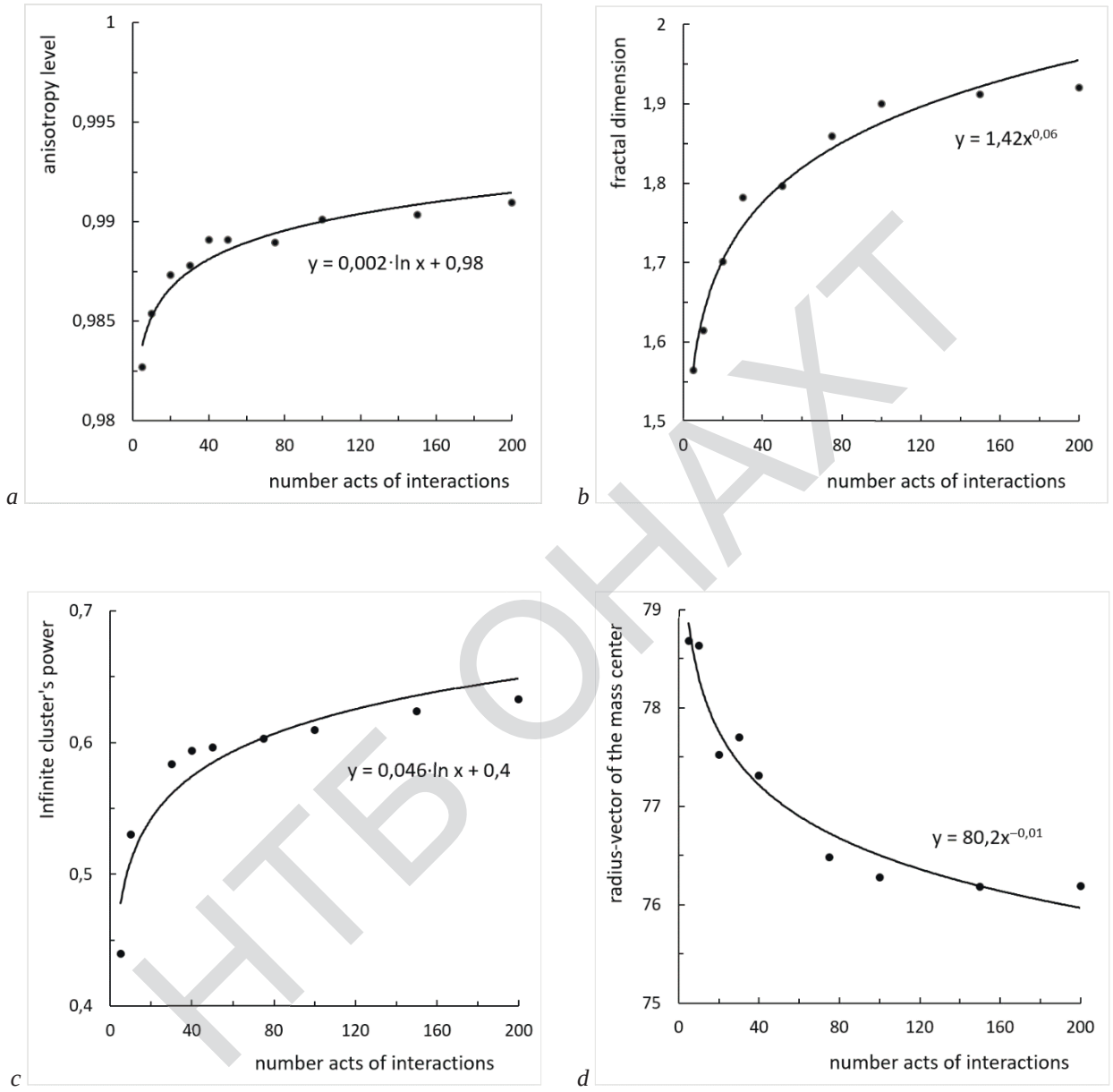
As a result of modeling using SCCM, analytical formulas for the dependencies of the above cluster system parameters on the initial simulation conditions and corresponding graphs were obtained. Some of them are shown at Pict.1.

The developed program complex allows to solve the following tasks:

- to calculate the parameters of model clusters, statistics of the distribution of clusters in the percolation field, to approximate experimental data, to obtain analytical formulas for dependencies, and to plot graphs;

- to study synergetic and physical mechanisms of the genesis of the structure of clusters and the possibilities of influencing them with the visualization of particle coagulation processes, the clustering of particles, the appearance of a percolation cluster;

- to study the influence of randomness on the types of model clusters, their structure and properties, to reveal the role of ordering factors and interparticle interaction at concentration phase transitions; to study, therefore, the structure of solids in intermediate asymptotic.



Pict.1. Dependence of the anisotropy level of clusters (*a*),
of fractal dimension (*b*), of the power of an infinite cluster (*c*), of the radius-vector of the center of mass (*d*)
on the number of particles generated in each iteration under the interaction law $1/R^2$

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