MODIFICATION OF THE RLA MODEL FOR PRESENTING A CLUSTER SYSTEM OF A COMPOSITE MATERIAL WITH A FRACTAL FILLER STRUCTURE

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I. INTRODUCTION

In [1 - 4], the quantitative characteristics of the spatial distribution of filler-copper particles in the matrix of a composite material based on polytetrafluoroethylene were investigated and determined using images of the surface obtained by optical microscopy methods. To determine the quantitative parameters of the structure of clusters, the method of cluster recognition based on threshold segmentation (Otzu method) was applied. Analysis of the distribution structure of copper particles in a polymer matrix at filler concentrations in the range of 1-20 wt. % shows that the structure of the filler forms clusters can be described within the reaction-limited aggregation (RLA) model. It was found that the fractal dimensions of the profile of the selected segments of copper clusters in the polytetrafluoroethylene matrix are in the range from 1.65 to 1.72 with a change in the mass concentration of copper from 1% to 20%. The fractal dimensions of the profile of the clusters, the structure of which was calculated within the framework of the RLA model (for three-dimensional lattices), vary from 1.62 to 1.72 when the probability of adhesion of a diffusing particle and cluster particles in the adhesion zone changes from 0.2 to 1. The fractal dimensions of the profile of the clusters, the structure of which was calculated within the framework of the RLA model (for three-dimensional lattices), vary from 1.62 to 1.72 when the probability of adhesion of a diffusing particle and cluster particles in the adhesion zone changes from 0.2 to 1. Such a parameter of the RLA model, as adhesion probability, can serve as a link between the fractal dimension of the cluster profile and its mass fractal dimension.

In accordance with the RLA model, one seed particle of the cluster is placed in the space under consideration, and then one new particle is added to the space. Each new particle moves according to the law of random walks. If a particle reaches the boundary of space, it is reflected from it. The particle continues to move until it is in the vicinity of one of the cluster particles. Further, the diffusing particle is attached to the cluster in accordance with the given probability of adhesion of the diffusing particle and the configuration of the cluster particles in the adhesion zone. If a diffusing particle joins a cluster, then the next particle is launched into space. If the attachment of the particle to the cluster did not occur, then the particle continues to move according to the law of random walks. Thus, a cluster is formed [5–7].

II. DESCRIPTION OF THE MODEL AND OBTAINED RESULTS

One of the options for modifying the RLA model is the condition for the termination of cluster growth. Usually, in the RLA model, the condition for the termination of cluster growth is that the cluster reaching the boundaries of the region. However, this condition can be changed by setting a finite amount (volume concentration) of primary particles from which a cluster is formed. Calculations, provided that the cluster reaches the boundaries of the region, show that the volume concentration of particles corresponds to 2%. The volume concentration of primary particles is related to the mass concentration of copper in the matrix of the composite material based on polytetrafluoroethylene and can be another parameter for comparing real clusters and model objects.

Real physical systems usually consist of several clusters (cluster system). In order to obtain a model of such a system, the RLA method can also be modified. In our case, unlike the RLA model, during the clustering process, seed particles are randomly added that do not move over the region and from which clusters can be formed. Also, during the clustering process, in accordance with the RLA model, particles are sequentially launched that diffuse over the area. If a diffusing particle enters a cell next to a cluster, then, depending on the adhesion probability, it either joins the cluster or continues to diffuse over the region. Thus, it is possible to build a cluster system. In this work, the RLA model was modified to study the properties of the cluster system in the range of the volume concentration of particles from 2 to 5% and the probability of adhesion of diffusing particles and cluster particles in the adhesion zone from 0.2 to 1.

In this case, an informative characteristic of fractal clusters of the system can be their average fractal dimension. Calculations have shown that the average fractal dimension of clusters in the system corresponds to the fractal dimension of clusters, the structure of which was calculated within the RLA model with the corresponding probability of adhesion of diffusing particles and cluster particles in the adhesion zone.

A computational experiment to determine the mutual influence of the adhesion probability and the volume concentration of particles on the formation of fractal clusters in a cluster system was carried out in accordance with the second-order orthogonal central compositional plan (OCCP) [8]. As a result of a computational experiment in accordance with the OCCP, the dependence of the mass fractal dimension of clusters from the volume concentration of particles and the probability of diffusing particles adhesion and cluster particles in the adhesion zone was obtained:

$$D = 2{,}524 + 2{,}167\ n - 0{,}385\ P + 0{,}5\ nP + 0{,}175\ P^2 \tag{1}$$

where D is the average mass fractal dimension of clusters, n is the volume concentration of primary particles, P is the probability of adhesion of diffusing particles and cluster particles in the adhesion zone.

III. CONCLUSIONS

The paper proposes a modification of the RLA model to study the properties of a cluster system. A computational experiment to determine the mutual influence of the adhesion probability and the volume concentration of particles on the formation of fractal clusters in a cluster system was carried out in accordance with the second-order orthogonal central compositional plan. As a result of the computational experiment in accordance with the OCCP, an equation was obtained for the dependence of the mass fractal dimension of clusters on the volume concentration from 2 to 5% and the adhesion probability of diffusing particles and cluster particles in the adhesion zone from 0.2 to 1. The developed methods for modeling a cluster system can be used to present the structure of the filler in composite materials and predict the physical properties (thermal conductivity) of composite systems.

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