http://dx.doi.org/10.35596/1729-7648-2021-19-8-35-39

Original paper

UDC 541.1

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

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Submitted 19 November 2021

Abstract. The paper proposes a modification of the diffusion-limited aggregation model to study the properties of a cluster system. A computational experiment to determine the mutual influence of the sticking 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). As a result of a computational experiment in accordance with the OCCP, an equation was obtained for the dependence of the mass fractal dimension of clusters on the volume of particle concentration and the probability of adhesion of diffusing particles and cluster particles in the adhesion zone. This dependence was obtained in a range of volume concentration of particles from 2 to 5 % and the probability of adhesion of diffusing particles and particles of clusters in the adhesion zone from 0.2 to 1.

Keywords: polymer composites, cluster system, fractal dimension, RLA models.

Conflict of interests. The authors declare no conflict of interests.

For citation. Belko A.V, Babarika N.N., Zeylikovich I.S., Nikitin A.V. Modification of the RLA model for presenting a cluster system of a composite material with a fractal filler structure. Doklady BGUIR. 2021; 19(8): 35-39.

Introduction

Simulation methods can be used quite effectively along with experimental methods for studying the structure and properties of objects. The known methods (the diffusion-limited aggregation model and its modification) make it possible to fully describe the structure of single fractal clusters. At the same time, it is important to study the influence of a cluster system on the physical properties of the entire compositional system. Therefore, it becomes necessary to develop aggregation models for describing a system of fractal clusters (cluster system) in a range of dimensions observed in physical objects.

In [1–7], 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. The 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 out 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 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. This 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.

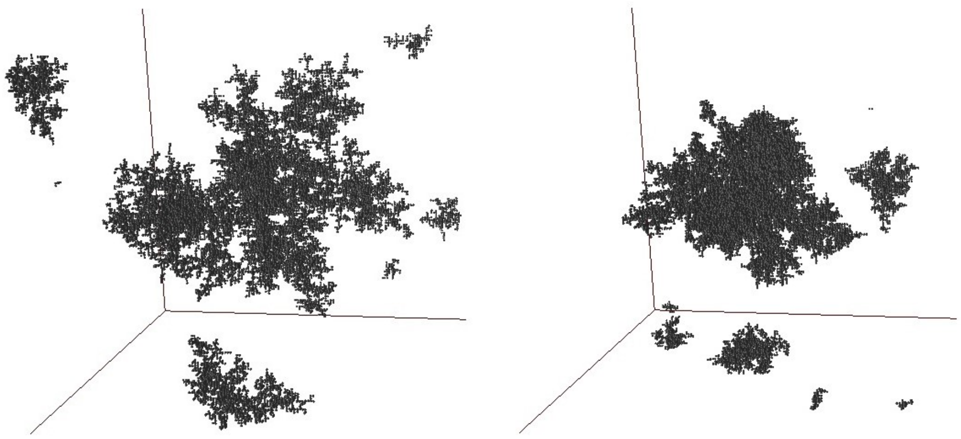
In accordance with the RLA model, one seed particle of the cluster is placed in the space under consideration, and then one new particle is added to the space. Each new particle moves according to the law of random walks. If a particle reaches the boundary of space, it is reflected from it. The particle 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 [8–10].

Methods of conducting experiment

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. The 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 so that they 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. The 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 diffusing particles and cluster particles adhesion in the adhesion zone. An example of fractal clusters of the system is shown in Fig. 1.



a *b*

Fig. 1. Cluster systems obtained within the framework of the RLA model on three-dimensional lattices at various sticking probabilities: *a* – 1.0; *b* – 0.2

Experimental results

Within the framework of the modified RLA model, a computational experiment to determine the effect of the volume concentration of primary particles and the probability of diffusing particles and cluster particles adhesion in the adhesion zone to their fractal structure in the cluster system was carried out in accordance with the second-order orthogonal central compositional plan (OCCP). OCCP refers to an "active" experiment in which the input actions are purposefully changed [11–12]. OCCP allows you to obtain a statistical model (empirical) of the research object. The object of the study is the response function, which connects the output parameter D (in our case, the mass fractal dimension) with the factors x_1 (volume concentration of primary particles) and x_2 (the probability of adhesion of diffusing particles and cluster particles in the adhesion zone). Numerical calculations for the three-dimensional case were performed at volume concentrations of primary particles from 2 to 5 % and the probability of adhesion of diffusing particles and particles of clusters in the adhesion zone in the range from 0.2 to 1. The OCCP allows obtaining a regression equation in the form of a full quadratic polynomial:

$$D = b_0 + b_1 x_1 + b_2 x_2 + b_{12} x_1 x_2 + b_{11}(x_1^2 - a) + b_{22}(x_2^2 - a)\,, \tag{1}$$

where x_1 and x_2 – are coded values of factors, a is a parameter that depends on a number of factors.

The maximum value of the volumetric concentration of primary particles is set at 5 % in the computational experiment corresponds to the coded value of factor 1, the minimum value of 2 % corresponds to the coded value of –1. Likewise, for the sticking probability, a maximum value of 1 corresponds to a coded value of 1, and a minimum 0.2 corresponds to –1. The values of the output parameter D (the results of repeating experiments D_1, D_2, D_3, D_4) corresponding to the coded values of the factors are presented in Tab. 1.

Table 1. OCCP experiment planning matrix

U	b_0	b_1	b_2	b_{12}	$b_{11}–a$	$b_{22}–a$	D_1	D_2	D_3	D_4
1	1	–1	–1	1	0,333	0,333	2,5	2,5	2,5	2,49
2	1	1	–1	–1	0,333	0,333	2,57	2,57	2,56	2,57
3	1	–1	1	–1	0,333	0,333	2,37	2,36	2,36	2,37
4	1	1	1	1	0,333	0,333	2,44	2,45	2,45	2,45
5	1	–1	0	0	0,333	–0,667	2,4	2,41	2,4	2,41
6	1	1	0	0	0,333	–0,667	2,48	2,47	2,48	2,47
7	1	0	–1	0	–0,667	0,333	2,54	2,53	2,54	2,53
8	1	0	1	0	–0,667	0,333	2,41	2,4	2,41	2,41
9	1	0	0	0	–0,667	–0,667	2,44	2,45	2,44	2,45

After carrying out a computational experiment in accordance with the OCCP technique, the hypothesis of the reproducibility of the experimental results was tested using the Cochran criterion [11, 12]. The calculated value of the Cochran test that equals to 0.125 turned out to be less than its critical tabular value equal to 0.403 for a 5 % significance level. In this case, you can start calculating the coefficients of the polynomial.

The calculation of the coefficients of the polynomial b_0, b_1, b_2, b_{12}, b_{11}, b_{22} in the regression equation (1) and their corresponding Student t-tests (respectively equal to 3132; 38.5; 65.8; 2.65; 1.75; 17) and subsequent comparison with the critical value of the Student's t-test equal to 2.05 for a 5% significance level showed that the coefficients of the polynomial b_0, b_1, b_2, b_{12}, b_{22} are significant. The b_{11} coefficient is insignificant. In this case, the mathematical dependence of the fractal dimension on the coded values of the factors (concentration of electrolyte counterions, potential) can be represented as:

$$D = 2.442 + 0.037x_1 - 0.063x_2 + 0.003x_1x_2 + 0.028x_2^2. \qquad (2)$$

At the next stage, the hypothesis about the adequacy of the constructed model was tested on the basis of the Fisher criterion [11, 12]. The value of the Fisher criterion was obtained – 1.62, which is less than the critical value (2.73 for a 5 % significance level). Based on the calculation, a conclusion was made about the adequacy of the regression model to the data obtained as a result of the computational experiment.

When passing from the coded values of the factors x_1, x_2 in the equation (2), respectively, to the factors expressed on a natural scale (volume concentration of primary particles, the probability of adhesion of diffusing particles and cluster particles in the adhesion zone), an equation was obtained for the dependence of the mass fractal dimension of clusters (D) on the volume concentration of primary particles (n), the probability of adhesion of diffusing particles and cluster particles in the adhesion zone (P) [12]:

$$D = 2.524 + 2{,}167n - 0.385P + 0.5nP + 0.175P^2. \qquad (3)$$

The developed methods for modeling a cluster system can be used to model the structure of a filler in composite materials and predict physical properties of composite systems.

Conclusion

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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Authors' contribution

Belko A.V., Babarika N.N., Zeyikovich I.S. and Nikitin A.V. performed the task for the study, obtained the results, and prepared the article in equal parts.

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