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ВПЛИВ РОЗПОДІЛУ ЧАСТИНОК ЗА РОЗМІРАМИ НА ФРАКТАЛЬНУ РОЗМІРНІСТЬ КОМПОЗИТУ НА ОСНОВІ ЗГЕНЕРОВАНИХ МОДЕЛЕЙ

У статті розглядається питання впливу розподілу частинок включень за розмірами на структурні характеристики (фрактальну розмірність) композитних матеріалів. Досліджено різні розподіли в широкому діапазоні відношень середньоквадратичного відхилення до математичного очікування. З'ясовано, що для практично значущих випадків, коли середньоквадратичне відхилення менше половини математичного очікування, такий вплив є малим і ним можна знехтувати.

Ключові слова: фрактальна розмірність, математична статистика, розподіл імовірностей, композит, структура, моделювання

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INFLUENCE OF PARTICLE SIZE DISTRIBUTIONS ON THE FRACTAL DIMENSION OF THE COMPOSITE BASED ON GENERATED MODELS

The paper deals with modeling of the influence of inclusion particle size distribution on the structural characteristics (fractal dimensionality) of composite materials. Different distributions in a wide range of ratios of standard deviation to mathematical expectation are studied. It was found out that for practically significant cases, when the standard deviation is less than half of the mathematical expectation, such influence is small and can be neglected.

Keywords: fractal dimension, mathematical statistics, probability distribution, composite, structure, modeling

Problem formulation

Composite materials play a key role in modern technology, offering unique mechanical, thermal and electrical properties that cannot be achieved with traditional materials. Their widespread use in various industries is due to the ability to customize the characteristics of such materials depending on the requirements of specific applications. Composites are based on a combination of matrix and filler, and their properties largely depend on not only the type of matrix material and filler, but also on the structural characteristics of the filler particles such as size, shape, and size distribution. The structural parameters such as particle packing density, pore distribution, and contact surfaces between particles have a direct influence on the physical and mechanical properties of the composite including strength, stiffness, and thermal conductivity. The fractal dimension can be a generalized indicator of the structural characteristics of a composite material [1], [2]. A natural question arises to what extent the structural characteristics of the composite (expressed through its fractal dimensionality) are affected by the type of particle size distribution of the filler used.

There are many theoretical and practical works and standards devoted to the analysis of statistical characteristics of grains, filler particles or other structural elements of composites [3], [4]. The issues of size distribution of powder materials or fillers of composites are considered much less widely, and the question of the influence of the distribution function on the structural characteristics of composites as such, in isolation from other physical and mechanical properties of the material, has not been practically considered.

Although there are works on particle size distributions, generally the distribution data are limited to values of D10, D50, and D90, i.e., diameters for which, among the whole set of powder particles, 10%, 50%, and 90%, respectively, have diameters smaller than the specified [4], [5]. In papers that attempt to more accurately describe the type of distributions, it is usually concluded that the actual distributions can best be described as a lognormal distribution, a gamma distribution, or a Weibull distribution with appropriate parameters [6], [7].

The objective of the present work is to study the degree of influence of the type of particle size distribution on the fractal dimensionality of a composite as its generalized structural characteristic.

Methodology of the computational experiment

The model of spherical particles randomly distributed in a cube with a side of 1260 pixels with a given distribution of particles by size was chosen as a model of composite material. Based on what has been said above about the results of practical study of powder particle size distributions, the most common distributions, namely Weibull, lognormal, gamma distributions (as well as normal and uniform distributions for comparison) were selected as model distributions. In the case of normal distribution, negative generated

values were discarded, in the case of uniform distribution, the parameters were limited to those that did not lead to the generation of negative values of the random variable were limited).

In order to study the influence of the type of particle distribution on the fractal dimensionality values, the parameters of the distributions were selected such that the mathematical expectation of the particle size μ and dispersion σ^2 would have the same values:

$$\mu = E[r] = \int_0^{\infty} rf(r)dr, \quad \sigma = \sqrt{E[r^2] - E[r]^2} = \sqrt{\int_0^{\infty} r^2 f(r)dr - \mu^2} \quad (1)$$

To eliminate the influence of other factors, especially the influence on the fractal dimensionality of the density of filling of the investigated volume, the studies were carried out for two different values of filling — 10 vol.% and 20 vol.%.

Based on the similarity principle, the influence of the average particle size can only occur due to edge effects of particle placement in the generated model (absence of particles crossing the edges of the cube has some influence on their distribution near the edges of the cube); to account for this, we conducted studies for two different average particle radii, 20 and 50 pixels.

For each mean value, generation was performed for the ratio of standard deviation to the mean, ranging from 0.01 to 5. Generation of the model sphere-filled cube was performed according to the method described in [8], and the calculation of fractal dimensionality — using the box counting method [9], [10]. To obtain reliable results, generation of 10 model objects was performed followed by averaging of the calculated fractal dimension.

Results and discussion

The computational results for the fill density of 10 vol.% and average radii of 20 and 50 pixels are shown in Fig. 1.

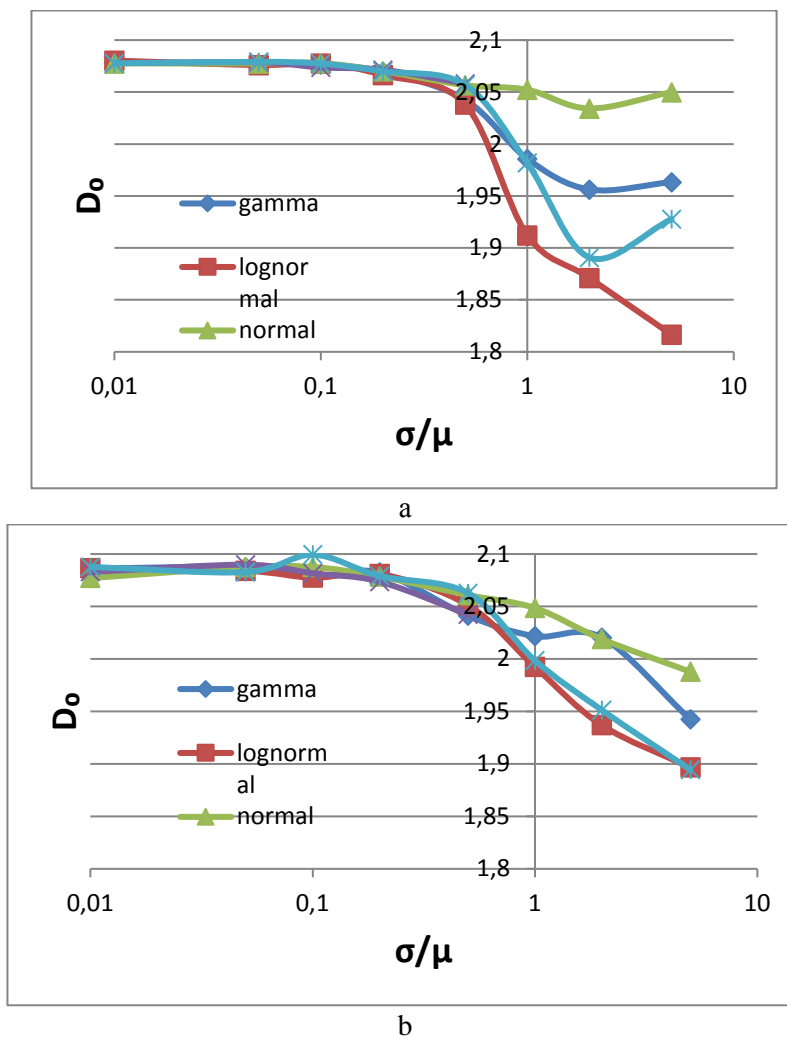


Figure 1. Fractal dimensions for different distributions as a function of the ratio of standard deviation to the mean for 10 vol.% occupancy and mean radius of (a) 20 and (b) 50 pixels

The results for 20% occupancy are shown in Figure 2.

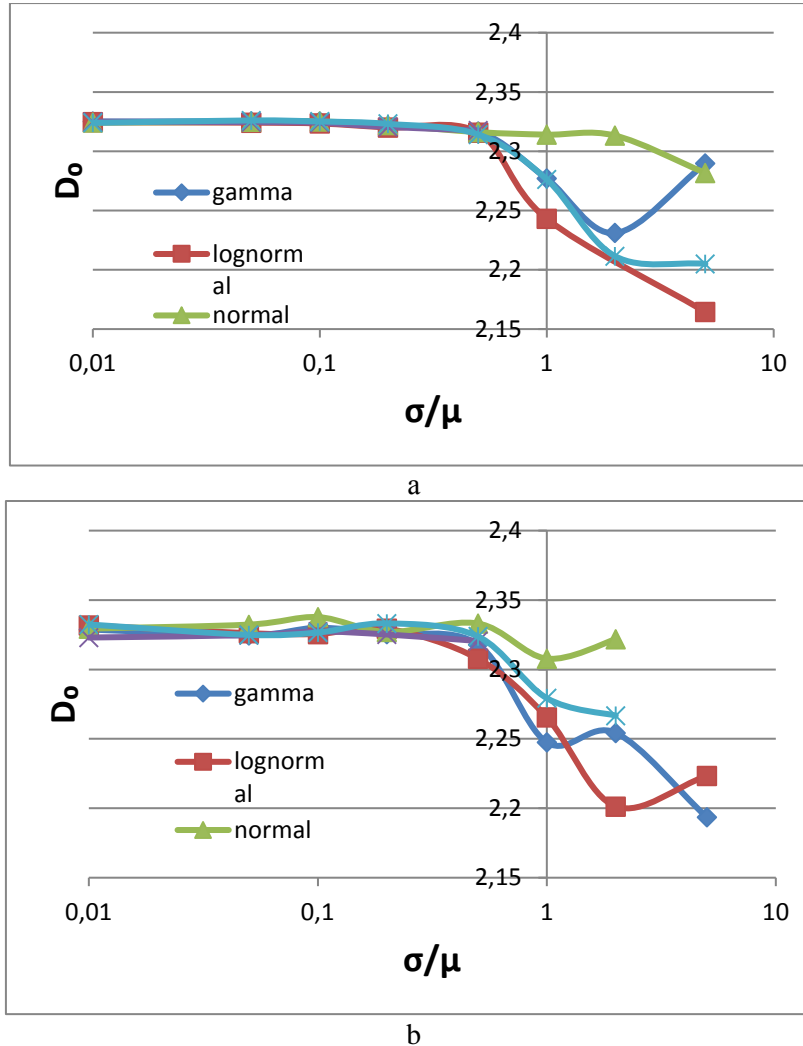


Figure 2. Fractal dimensions for different distributions as a function of the ratio of standard deviation to the mean for 20 vol.% occupancy and mean radius of (a) 20 and (b) 50 pixels

As can be seen from the obtained graphs, the results for values of σ/μ smaller than 0.5 depend only on the cube occupancy, and do not depend on the ratio of standard deviation to the mean value, nor on the type of distribution of the sphere sizes.

At values of σ/μ larger than 0.5, a divergence of D_0 values for different distributions is observed. Certain disordered behavior of the fractal dimension dependence on the value of σ/μ can be explained by the fact that at large values of σ/μ the distribution functions have a large "right tail" (see Fig. 3), i.e., many spheres are comparable in size to the size of the model cube, which leads to significantly different generated models and, as a consequence, a scatter of the calculated value of the fractal dimension. A more detailed study of the fractal behavior for such large values of σ/μ is possible at the cost of significantly increasing the size of the models and the required computational resources. However, since experience shows that experimental values of σ/μ for real powders do not go beyond the [0; 0.5] range, such a study is primarily of theoretical interest.

The graphs of the distribution density functions for values $\sigma/\mu < 0.5$ (Figure 2), demonstrate obvious similarity. It is theoretically possible to construct artificial distributions with the same values of mathematical expectation and standard deviation, which would demonstrate a significant difference from the bell-shaped form of the distribution density function. However, as shown by the above-mentioned works [4-7], such distribution of particle sizes in real powder technologies does not occur, and, therefore, is of no direct practical value.

Thus, the study results demonstrate that fractal characteristics across a broad range of particle size distributions are primarily determined by particle occupancy within the composite. The similarity in scaling

suggests that the average particle size, while impacting the composite's physical properties, has a lesser effect on its structural characteristics. Therefore, further research should explore the influence of particle size distributions on multifractal characteristics and the structural properties of selected grain boundary systems.

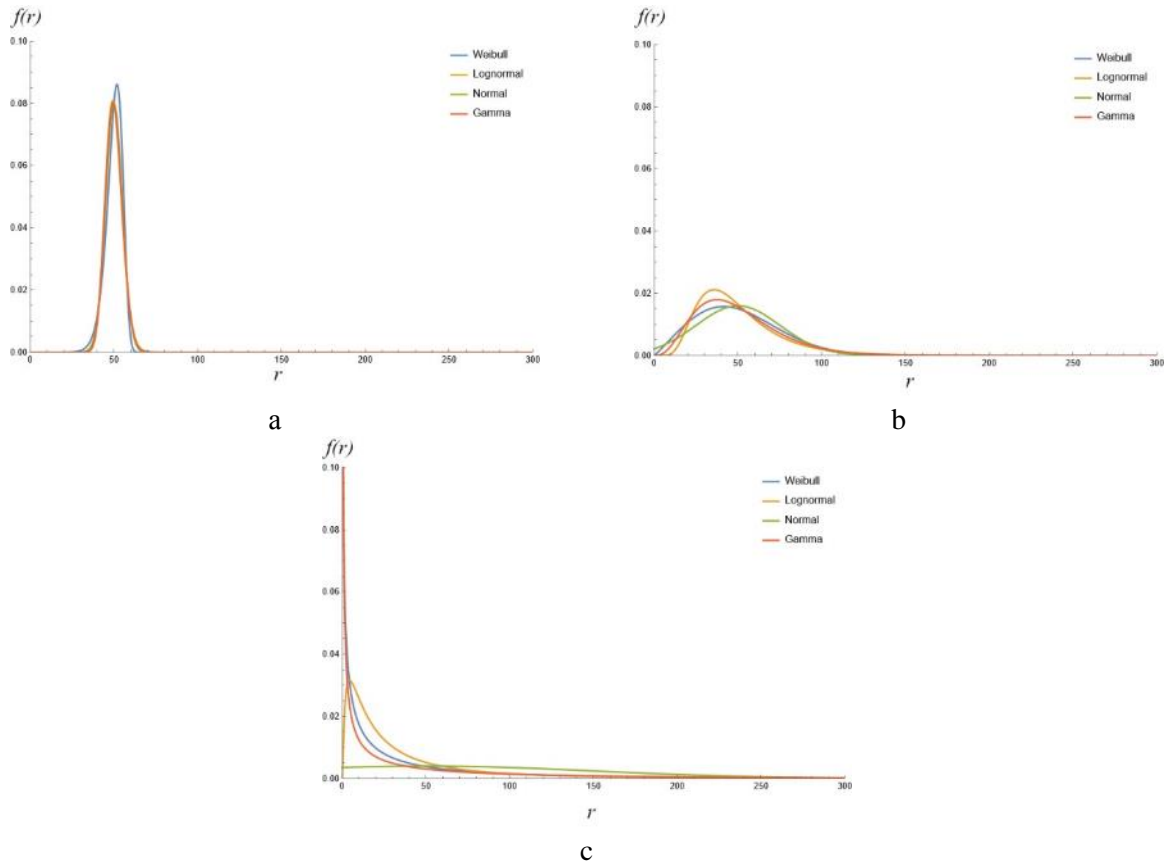


Figure 3. Density functions of different distributions for $\mu = 50$ and σ/μ equal to a) 0.1; b) 0.5 and c) 2.

Conclusions

In this work, a study of the effect of powder particle size distribution on the structural properties of composite materials has been carried out. It is shown that in cases when the ratio of the distribution standard deviation to the mathematical expectation does not exceed 0.5, the influence of both the distribution and the value of the mentioned ratio on the structural characteristics (fractal dimension) is small. In situations of practical interest, the key factor that determines the bulk fractal dimension of a composite can be considered to be the filler occupancy of the composite; the study of the factors affecting the fractal dimension of the boundary system is a topic of further research.

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