Fractal analysis of disperse systems

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Abstract. A method for determining the fractal dimension of metallic and nonmetallic disperse systems which is based on measuring the masses of formed clusters of various sizes was developed. The different character of the change in the fractal dimension with a change of the true density of the particles of the disperse phase of metallic and nonmetallic systems was shown. The effect of the packing density of powder materials when poured under free embedding on their fractal dimension was evaluated. It is proved that the increase in packing density leads to an increase in the fractal dimension. The effect of the shape of the particles of the dispersed phase on the fractal dimension of disperse systems, characterized by the inequality of axes factor is studied. It was found that the decrease in the standard deviation during the determining of the fractal dimension due to the developed method is caused by the increase in the fractal dimension of the cluster because of the influence of the size and factor of the inequality of axes of the particles of the dispersed phase.

1. Introduction
One of the urgent problems of modern materials science is the creation of new composite materials with specified properties.

The structure of multicomponent composite materials is a complex statistical system of interacting macro- and microparticles. They are different in their physico-chemical and structural-mechanical properties. Due to this fact, an important role in the formation of the structure and properties of composites is taken by the geometric structure of their components, which determines the course of the processes of the formation of structure.

Most real disperse systems are disordered structures. One of the approaches to their modeling is the use of the apparatus of fractal geometry [1-5]. In this case, both regular fractals as well as stochastic ones are used. Regular fractals have a geometrically the exact structure and are constructed due to deterministic algorithms. The greatest interest in describing the kinetics of processes occurring in disperse systems, obtaining values which characterize the degree of filling of a porous space, the determining of the specific content of individual phases, and estimating the area of mutual contact of the surfaces of their structural components is represented by stochastic fractals.

Fractal analysis is widely used in the study of materials and the development of processes for their production. It is proposed to use the fractal dimension as the main parameter for analyzing nanoparticles synthesized by various methods [6]. Analysis of two-dimensional images of asphalt mixtures allowed to develop a method of control from the structure [7]. Fractal analysis is used to assess the effectiveness of milling Li$_2$TiO$_3$ used as a battery [8]. Based on fractal analysis, the effect of sonication on the structure
of ZrO particles is shown [9]. Fractal analysis of diatomite is carried out after various modes of its heat treatment [10].

In the majority of works in which the authors apply fractal analysis, the effectiveness and informativeness of such methods are noted. However, researchers are faced with the problem of the occurrence of significant errors in the measurement of the fractal dimension of materials caused by changes in their physico-mechanical characteristics.

The purpose of this work is a fractal analysis of disperse systems in the form of bulk materials of various nature and the revealing of the patterns of variation of fractal dimension under the influence of variations of the structural characteristics and physical properties of both individual components and their aggregate.

2. Materials and methods of research

The methods for determining the fractal dimension are based on the self-similarity hypothesis of the explored system, i.e. the similarity of its structure is invariant with a change in scale [1-3, 11-13].

Bulk materials are multifractal objects [1, 14, 15]. This means that they are characterized by a spectrum of fractal dimensions. Mostly it is caused by the change of the concentration of the solid and gas phases in the layer with the increasing of cluster size. It’s obvious that the wider the range of scrutinized materials volumes is, the stronger the degree of influence on the fractal dimension of the packing density will be (because of the increase of the pressure of the overlying layers on the lower layers), and the influence of such quantities as the true density of the material of the particle, their shape and the factor of inequality of axes, which are not changed with the change of the volume of clusters, is weakening. As a result, in order to achieve the goal, set in our work, it is expedient to study homogeneous fractal subsets, the feature of which is the decreasing character of the dependence of the concentration of the solid phase of the cluster on its size

\[
\frac{V_s}{V_{cl}} = \left( \frac{d_p}{L} \right)^{d-D},
\]

where \(V_s\) – volume of the solid phase; \(V_{cl}\) – total volume occupied by the cluster; \(d_p\) – average diameter of the particle; \(L\) – size of the cluster; \(d\) – topological (Euclidean) dimension of physical space; \(D\) is the fractal dimension.

In figure 1 the density distribution of the formed clusters depending on their sizes is shown. The decreasing character of dependencies indicates their uniformity and fractal behavior.

![Figure 1. Dependencies of fractal cluster density on their size.](image)
Measurement of the concentration of the solid phase in a heterogeneous system is a complex experimental task because of its disorder and various structural features of the particles of the material. Let’s write an expression (1) in the form

\[ \frac{\rho_{cl}}{\rho_{p}} = \left( \frac{d_{p}}{L} \right)^{d-1}, \]  

(2)

where \( \rho_{cl} = \frac{m}{V_{cl}} \) is the density of the cluster; \( \rho_{p} = \frac{m}{V_{p}} \) – the density of the cluster particle material; m is the mass of the cluster.

After logarithming the left and right sides of the expression (2) will be

\[ \ln \left( \frac{\rho_{cl}}{\rho_{p}} \right) = (d - D) \ln \left( \frac{d_{p}}{L} \right), \]

so with the consideration of the statistics of the distribution of the densities of N clusters due to their dimensions, there will be such the mathematical expectation of the value of the fractal dimension

\[ D = d + \frac{1}{N} \sum_{i=1}^{N} \ln \frac{\rho_{cl}}{\rho_{p}}. \]  

(3)

Dependence (3) links the density and diameter of particles in the solid phase of the disperse system, as well as the density and size of the cluster formed from the cluster with a fractal dimension. On the basis of the obtained dependence, a method of determining the fractal dimension was created. It includes the following main steps:

- formation of a cluster of a given size \( L_{i} \) by pouring of the researched material into a capacity of \( L_{i} \);
- measuring the mass \( m_{cl_{i}} \) of the formed cluster and calculating its density \( \rho_{cl_{i}} = \frac{m_{cl_{i}}}{L_{i}} \);
- iteration of previous operations for a number of different sizes of \( L_{i} \);
- calculation of the fractal dimension by the formula (3).

During the research, metal powders (copper (Cu), nickel (Ni), cobalt (Co), iron (Fe), tin (Sn)) and non-metallic bulk materials (wollastonite (Wo), sand (Sd), marshalit (M), aluminium hydroxide (Al(OH)3), graphite (G), shungit (Sh), coal (C1, C2)) with different sizes and shapes of the particle (factor of inequality of axes F) were used. The sizes and the shape of the particles of the test material using optical microscopy techniques were defined.

### 3. Results of experimental research and its explanation

The results of determining the fractal dimension according to the method described above are presented in Table. 1. Simultaneously with the fractal dimension, calculated by formula (3), its standard deviation \( \sigma \) was determined:

\[ \sigma = \sqrt{\frac{\sum_{i=1}^{N} (D_{i} - \overline{D})^2}{(N-1)}}. \]

In conformity with the purpose of the research, the effect of the true density of the particle material on the fractal dimension of the disperse system was analyzed. The data analysis of the table 1 shows that the nature of the change in the fractal dimension depending on the function of the true density for metallic and nonmetallic materials is different: as the true density increases, the fractal dimension of nonmetals increases, and the metal decreases.

Original research, the results of which are in article [16], shows that the different nature of dependence \( D(\rho_{p}) \) is linked with the influence of the degree of covalence of chemical bonds [17] (in case of metal powders) and also with ionic component of the chemical bond (in case of non-metallic materials).
Table 1. Results of determination of fractal dimension of disperse systems.

| Material | \(d_p (\mu m)\) | \(D\) | \(\rho_p (g \text{ cm}^{-3})\) | \(\sigma\) | \(\frac{\rho_{cl}}{\rho_p}\) | \(F\) |
|----------|----------------|-------|-----------------|--------|----------------|-------|
| Cu       | 100            | 2.699 | 8.93            | 0.025  | 0.21           | 2.30  |
| Ni       | 60             | 2.801 | 8.80            | 0.012  | 0.32           | 1.00  |
| Co       | 60             | 2.747 | 8.75            | 0.022  | 0.23           | 2.00  |
| Fe       | 160            | 2.793 | 7.85            | 0.015  | 0.33           | 1.00  |
| Sn       | 100            | 2.907 | 7.28            | 0.005  | 0.57           | 1.00  |
| Wo       | 30             | 2.826 | 2.94            | 0.005  | 0.31           | 4.00  |
| Sd       | 100            | 2.871 | 2.65            | 0.005  | 0.50           | 1.36  |
| M        | 30             | 2.837 | 2.62            | 0.008  | 0.34           | 1.00  |
| Al(OH)_3 | 7              | 2.821 | 2.42            | 0.002  | 0.23           | 1.25  |
| G        | 100            | 2.717 | 2.23            | 0.016  | 0.22           | 2.00  |
| Sh       | 1900           | 2.692 | 2.10            | 0.058  | 0.48           | 2.20  |
| C1       | 1950           | 2.555 | 1.80            | 0.060  | 0.30           | 2.37  |
| C2       | 2000           | 2.423 | 1.80            | 0.130  | 0.27           | 2.50  |

In the technological processes connected with the compacting of powdered materials, an important parameter determining the quality of the final product is the packing density of the material [18]. The packing density is defined as the ratio of the bulk density of the material to its true density \(\frac{\rho_{cl}}{\rho_p}\) in table 1. The densities of the formed packages do not exceed the maximum value of 0.64 for the free-flowing.

As a result of approximation of experimental data, reflecting the dependence of the fractal dimension on the packing density, such expressions were obtained:

- for non-metallic materials:

\[
D = 2.588 + 0.408 \cdot \frac{\rho_{cl}}{\rho_p};
\]  

(4)

- for metallic materials:

\[
D = 2.661 + 0.349 \cdot \frac{\rho_{cl}}{\rho_p}.
\]  

(5)

The dependence between (4) and (5) shows that despite the nature of the material, its fractal dimension is going up if there is an increase of the packing density.

The adequacy of the subjection linking the fractal dimension with the packing density is confirmed by the fulfillment of the boundary conditions: on the one hand, with \(\frac{\rho_{cl}}{\rho_p} \rightarrow 1\) the material is a monolithic solid body with zero porosity that does not possess fractal properties with a topological dimension of 3; on the other hand, a decrease in the packing density leads to an approximation of the fractal dimension to a value which is suited to the dimension of the percolation cluster at the percolation threshold \(D \approx 2.524\) [11, 19].

The deviation of the experimental data (Table 1) from the approximating subjections is linked with the essential differences (in nonmetallic materials) in the sizes of the particles of the dispersed phase and their shape.

From a geometric point of view, the fractal dimension of the bulk material characterizes the degree of filling of space with it. It’s obvious that the shape of the powder particles which is characterized with
the inequality of axes factor, will influence not only the degree of filling of the space, but also the fractal dimension.

To assess the degree of influence of the particle shape of bulk materials on the fractal dimension, approximation dependence was received due to the table 1:

\[ D = 3.086 + 0.18 \cdot F \]  \hspace{1cm} (6)

The inequality of axes factor \( F \) was obtained as the ratio of the largest diameter (linear size) of the particle to its smallest diameter (linear size).

For finding the dependence (6), materials of different nature with the same average particles size \( (d_p = 100 \, \mu m) \) were chosen.

Analysis of the obtained pattern (6) shows, that with the same particle size, without reference to the nature of the material, the fractal dimension increases when particles approaches to the spherical shape and when the factor of inequality of axes decreases.

In Figure 2 the link between the mean value of the fractal dimension and its standard deviation is shown.

![Figure 2. Relation between mean value of fractal dimension and its standard deviation.](image)

An increase in the standard deviation with a decrease of the fractal dimension of the material has a systematic character, which is primarily caused by an increase of the extent of solid particle boundaries caused by an increase of the particle size of the dispersed phase and, secondarily, with an increase of factor of inequality of axes of particles.

4. Conclusion

As a result of the research, the influence of the physico-mechanical properties and structural characteristics of dispersed systems in the form of bulk materials on their fractal dimension has been studied. The dependence connecting the fractal dimension with the density and particle size of the solid phase of the dispersed system, as well as with the density and size of the cluster formed from it, was obtained.

It was established experimentally that the fractal dimension of non-metallic bulk materials increases with increasing particle density of the dispersed phase, and metal decreases. This is consistent with previous studies [16], which have shown that a decrease in the packing density of the crystal lattice with an increase in the degree of covalence of the chemical bond causes a decrease in the degree of filling of space with a cluster at the macro level and a decrease in the fractal dimension of metal powders. The growth of the fractal dimension and the increase in the density of non-metallic bulk materials is associated with a decrease in the degree of covalence and an increase in the degree of ionicity of their chemical bonds.

The dependences connecting the fractal dimension of dispersed systems with their packing density were obtained. It has been proved that, all other things being equal, the fractal dimension of disperse systems decreases with an increase of inequality of axes factor of their particles. The nature of the change
in the standard deviation in determining the fractal dimension of its average value, due to the influence of the particle size of the dispersed phase, as well as the factor of their inequality of axes, was established.

The obtained dependences can be useful in analyzing the sources of error arising from measurements of the fractal dimensions of various materials.

The results of the research can be used in the development of composite powder materials with predetermined properties, the choice of the optimal amount of injected modifying additives and fillers, and can also be used as the basis for creating new methods of control the physico-mechanical properties and structural characteristics of porous materials.

5. Acknowledgments
The reported research was funded by Russian Foundation for Basic Research and the administration of the Tambov region of the Russian Federation, grant No. 19-43-680003.

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