STATISTICAL CHARACTERISTICS OF ENERGY-SAVING COMPOSITES' STRUCTURE

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One of the main tasks of building materials science is the creation of multifunctional energy-saving materials for various purposes. The general strategy for the preparation of such compositions is based on obtaining the composition from the available component, which combines binding material, which, as a rule, has a high thermal conductivity, and one or more fillers providing heat-insulating properties [1]. As a special filler, air or other gases can be considered. Adding these components is provided by adding foam or blowing agents to the binder paste.

Particles of heat-insulating filler or pores that serve as a barrier to heat flow are surrounded by layers of relatively homogeneous material forming inter-porous gaps (Fig. 1).

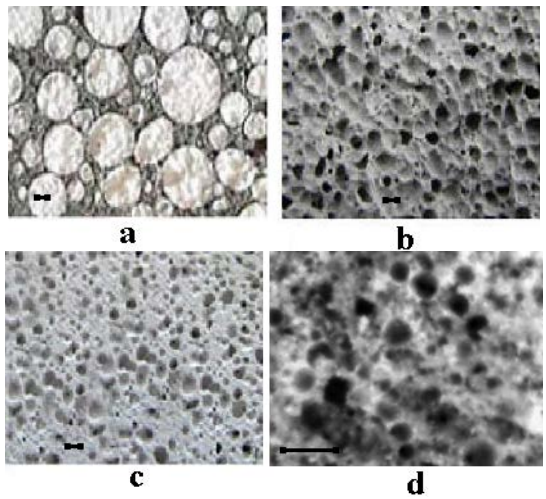

Figure 1. Examples of heat-insulating composites (scale – 1 mm): *a – polystyrene concrete, b – foam concrete, c – gas silicate, d – gypsum-pearlite composition*

When optimizing the thermal and strength properties of such composites, it is necessary to introduce the maximum amount of filler into the composite binder paste, approaching the percolation transition to the region of lower thermal conductivity [2], but not permitting a decrease in strength below the normative level (Fig. 2).

A study of the performance characteristics of heat-insulating composites shows that their thermal conductivity is largely determined by the density. This dependence is not, however, unique-the thermal conductivity of the material at a fixed density can be reduced by optimizing the structure. Structural optimization allows improving the strength characteristics, which makes it possible to introduce additional amount of heat-insulating filler into the composite, reducing the thermal conductivity of the material [3].

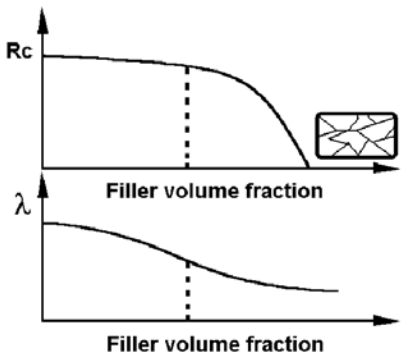

Figure 2. The task of optimizing the composition of heat-insulating material. The optimum proportion of the filler is indicated by a dashed line

This kind of optimization can be carried out in different ways, in particular, by selecting the granulometric composition of the components and adding structure-forming particles [4]. Therefore, the study of the heat-insulating composites' structure has not only theoretical, but also practical interest for building materials science.

The results given below are obtained by generalizing the data of the investigation of the structure of the plaster thermal insulation composite by the method of computer microscopy and image processing [5]. According to the proposed model, the structure of materials is represented by a set of interacting and transitioning into each other structural ensembles located quasiregularly. Each of them is a structure-forming particle or a pore surrounded by layers of interparticle (inter-porous) material formed under the influence of this particle (Fig. 3).

One of the methods for studying structural ensembles is based on optical-densitometric measurements. For this purpose, pore centers were automatically detected on micro-photographs with respect to the smooth sections of the sample

surface. From these centers, at equal angular distances from each other, segments were built up to the outer boundaries of the structural ensemble (in the case under consideration, the length of the segment was 1.6 mm).

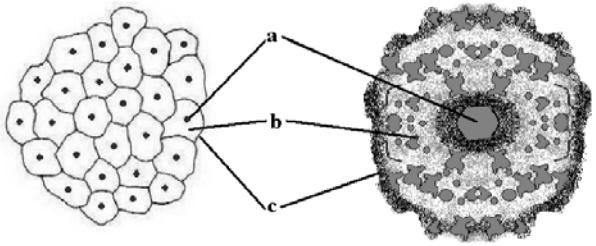

Figure 3. Model of the structure of heat-insulating composites: *a – structure-forming particle or pore, b – layers of interparticle (inter-porous) material, c – boundary of structural ensemble*

Optical densitograms were studied along each of these segments (Fig. 4).

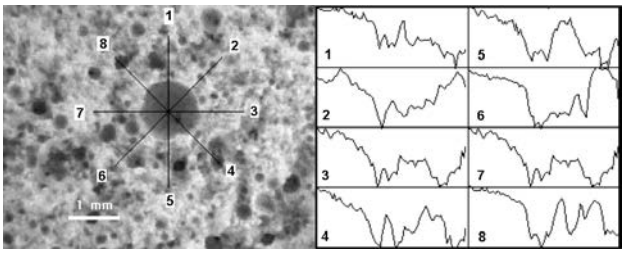

Figure 4. Results of densitometric analysis of a structural ensemble for eight directions

To obtain an objective estimate of the radial intensity allocation, the densitograms were averaged over the directions, and a radial intensity profile was constructed (Fig. 5-1). The number of

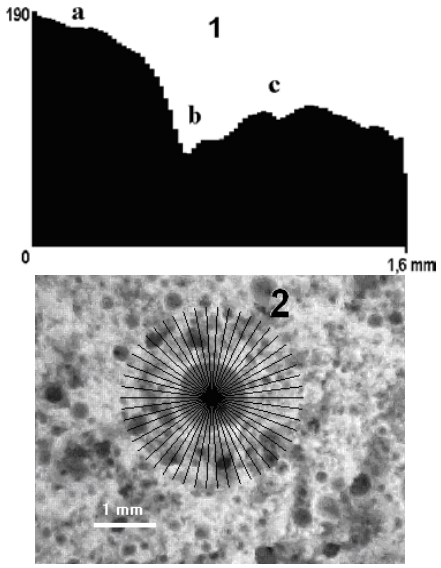

Figure 5. Densitometric study of pore structure: *1 – averaged radial profile of the structural ensemble (a – pore area, b – material compaction region, c – periphery of the structural ensemble); 2 – method for constructing an average radial profile*

directions is increased to 50 (Fig. 5-2) to improve the statistical reliability of the studies.

Near the pores the properties of the material are changed (Fig. 5-1, b), a region of high plastic deformations is formed here. Pore (or a structure-forming particle) has an active influence on the organization of the nearby material taking into account its geometric shape. From the system point of view, such particles can be considered a structural determinant [6], "imposing" a specific set of properties to the nearby material (Fig. 6).

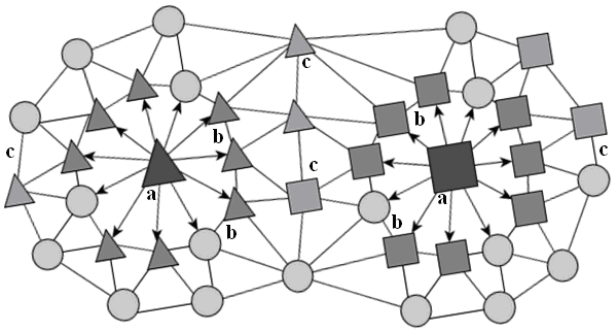

Figure 6. The principle of the structural determinant: *a – structure-forming particles, b – material regions near the interface, c – periphery of the structural ensemble*

Thus, it seems likely that the formation of structural ensembles from the structure-forming particle and the material with altered properties separated from this particle by the interface. With increasing characteristic dimensions of the research area, we move on to the structure formed by interacting and transitioning into each other structural ensembles. The study of this structure can also be carried out on the basis of computer microscopy and the method of statistical geometry [7, 8]. The method of the radial allocation function was used. The radial allocation function $g(r)$ is the main statistical characteristic of the degree of structural ordering in condensed systems in the theory of liquids and amorphous solids [9]. The radial function $g(r)$ shows how many times the probability $dw(r)$ of detecting a particle at a distance *r* from the central particle is larger for the allocation under consideration than for a chaotic particle allocation $dw_{dis}(r)$

$$g(r) = \frac{dw(r)}{dw_{dis}(r)} \qquad (1)$$

The spatial allocation of the pore centers on the chips of the samples of the heat-insulating composite was studied (Fig. 7, a).

The result of examining one of the samples, which is typical, is shown in Fig. 7, c. Here, by analogy with the theory of the liquid state [9], we can introduce the concept of coordination spheres corresponding to maxima.

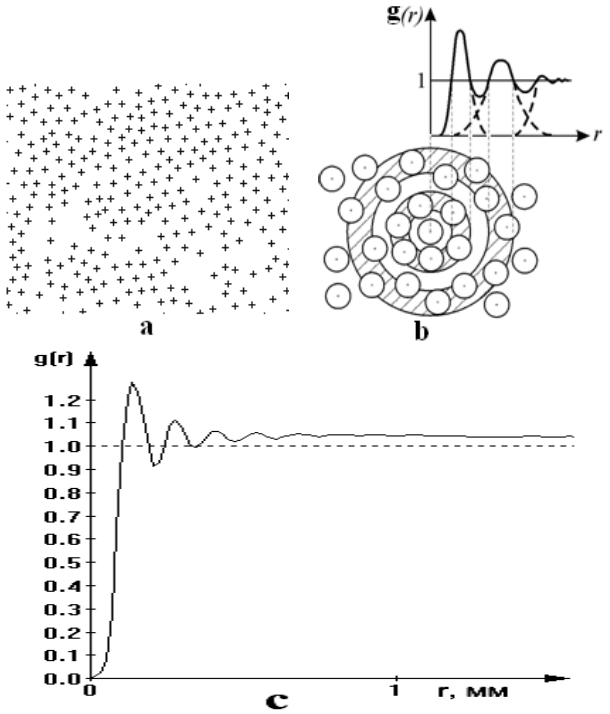

Figure 7. Studies of the allocation of pore centers using the radial allocation function: *a – allocation of pore centers on the cleavage surface of the composite (fragment), b - method of radial allocation functions for the liquid state, c - radial allocation function of the pore centers*

The corresponding distances are also called the radii of the coordination spheres. As in liquids (Fig. 7, b), the radial allocation function oscillates with distance (Fig. 7, c), which is evidence of the presence of short-range order interaction. Oscillations gradually decay, minor deviations from 1 at large r arise due to edge effects. Thus, the results of the investigation of the porous structure by the radial allocation function testify in favor of both the model under consideration (Fig. 3) and the quasiregular arrangement of the structural ensembles. Additional confirmation of the formation of structural ensembles can be obtained by analyzing the geometric characteristics of their filling the surface, reflecting the spatial distribution.

On the basis of point distributions, it is possible to construct the coverings of the plane by polygons – the Voronoi's decomposition [10] – and to study their statistical properties. For an arbitrary point from the system of points, we can specify a region of space, all points of which are closer to a given center than to any other center of the system. The set of such areas, constructed for each center of the system of points, generates a mosaic of polygons (the Voronoi's decomposition).

This decomposition was built around the pore centers for various samples of the material under study, and its geometric characteristics – polygon distributions over areas and perimeters – were investigated. The fragment of the decomposition for one of the samples, as well as the corresponding allocations, is shown in Fig. 8.

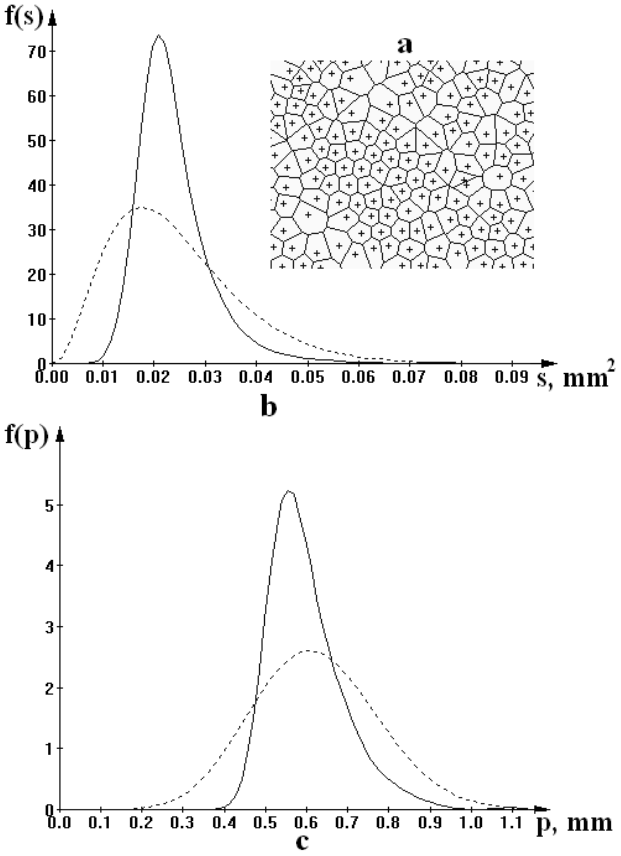

Figure 8. Voronoi's decomposition for the porous structure of the studied composite: *a – fragment of Voronoi mosaic for pore centers, b – allocation of Voronoi's polygons along areas, c – allocation of Voronoi's polygons along perimeters.* Dotted line - allocation for a random point system

The allocation of the areas and perimeters of the Voronoi's polygons is qualitatively coordinated, they describe the nonrandom, quasiregular arrangement of structural units, which corresponds to the hypothesis of structural ensembles. To interpret the general nature of the decomposition and its statistical properties, it can be assumed that each Voronoi's polygon approximates the spatial regions of influence of pores and structure-forming particles. In many cases, they will play the role of elements of a system of composite materials that determine the dynamics and structure of the

remaining elements (the structural determinants discussed above (Fig. 6)). The properties and structure of the rest of the material in the Voronoi's polygon are determined by their nature.

The influence of structure-forming particles and structural determination are clearly manifested in systems with a predominance of direct bonds. For the interaction of large pores with a material of total predominance, direct effects are not present - the surrounding material is able to influence on the geometric characteristics of pores and, in particular, its shape. As a result of the action of the set of causes (dissolution, transport and crystallization of the gypsum binder, surface effects of water interaction from the binder paste and filler, transfer processes, changes in the volume of composite areas, the appearance of internal deformations), the pores deform and, instead of the classical spherical, take the wrong shape, however, it is convenient to approximate by an ellipsoid [11]. On the sections and chips of material samples they are displayed by ellipses. The local anisotropy of the porous structure is investigated-the allocation of the ratios of the large and small semi-axes of approximating ellipses for each pore in the plane of one of the samples (Fig. 9) and the allocation of pores over the corners. It can be seen from the figure that for the sample under study the corresponding ratio is sufficiently large, which is one of the signs of an anisotropic porous structure.

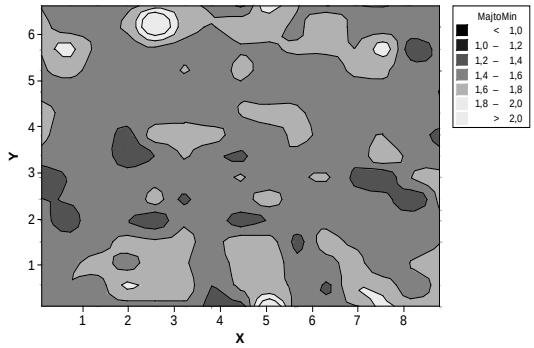

Figure 9. Characteristics of the pores' ellipticity (the ratio of the semi-axes of the approximating ellipse, MajtoMin) in the plane of the sample

The second sign of anisotropy, which is of interest in the design of thermal insulation materials, is the allocation of the orientation of the pores relative to the direction of the heat fluxes (Fig. 10).

The thermal resistance of the samples of the material, other things being equal, is higher in the case of a porous structure orthogonal to the lines of the average heat flux, due to the spatial organization of the material between the porous gaps.

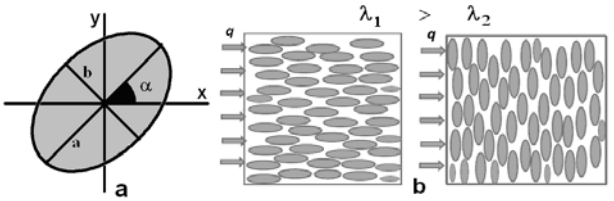

Figure 10. Orientation of the pores (a) and its effect on the thermal conductivity of the material (b)

Based on the computer microscopy data, a histogram of the observed orientation of the pores was constructed (Fig. 11, a), and the spatial distribution of the orientation angles was studied (Fig. 11, b). An investigation of this distribution was carried out by the grid method of 2-D interpolation [12].

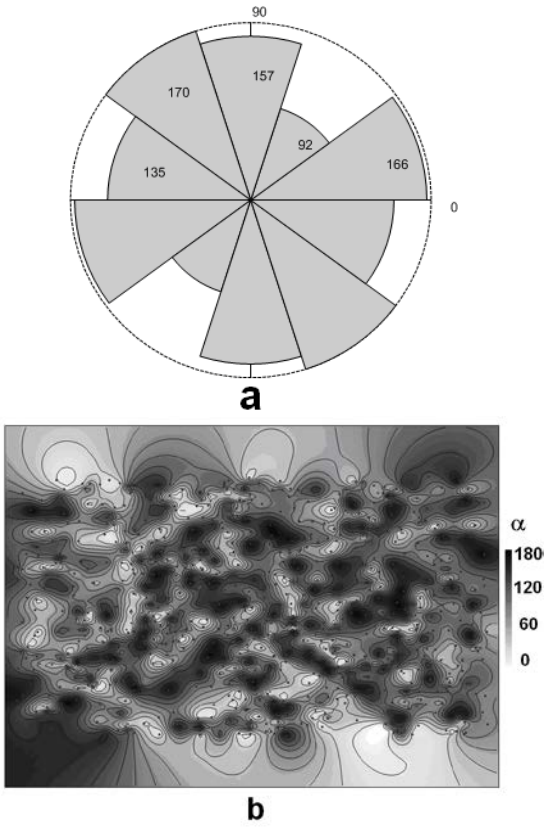

Figure 11. Quantitative characteristics of the spatial orientation of pores; *a - histogram of the allocation of pores along the directions, b - spatial allocation of the orientation angles*

The grouping of neighboring pores with a similar spatial orientation is visually determined (darkening in Figure 12, b), which is another evidence of the formation of pore ensembles. Processes of structure formation of a local character obviously cause internal deformations of a similar kind, imparting the same orientation to the corresponding pores. A high degree of anisotropy, corresponding to significant local deformations of the material, indicates the intensity of structural-

mechanical processes. These phenomena are possible near the surface of samples and products, grains of large filler, areas of significant contraction and expansion of the composite. The formation of a porous structure with a characteristic orientation and anisotropy is due to the composition and, to a large extent, the technological factors of fabricating the material.

Porous structure is the material basis for the manifestation of performance characteristics: strength, heat conductivity, adhesion properties and sound permeability. A purposeful organization of the structure of the material is a method of controlling its properties.

The main structural feature considered here by several methods is the tendency of the formation in the material of organized interpenetrating volume units - structural ensembles. Their parameters, such as the radii of the coordination spheres, the degree of compaction of the peripheral material, the distribution over the areas, depend significantly on the composition of the composite and, thus, can act as a „*intermediary*" of the effect of prescription and technological factors on performance characteristics.

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