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Investigation of the Structural Topological Characteristics of Mechanically Activated Sialic Raw Materials

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Abstract. This work presents the results of investigations of the topological characteristics of quartz raw materials of various mineral compositions crushed to the critical state of the dispersed layer under which the shape of the particles and the action of the electrostatic repulsion forces change.

Introduction

Currently, one of the main areas of scientific development is the optimization of cement composites and mortars in order to obtain the best strength indicators. Today, a promising and most effective way to increase the efficiency of composites is the use of composite binders: fine-grained multicomponent cement (FGMC) and low water demand binder (LWDB). The production of such highly disperse and mechanically activated binders leads to a reduction in cement consumption in the material and an increase in its performance characteristics [1–9]. However, in the absence of the necessary knowledge of the interrelation of the structure, the physico-topological state and the structure with the properties of the material, it is impossible to fully predict the behavior of the material under operating conditions. For example, it is known that high-strength concretes with low water/cement ratio (W/C) have increased brittleness and reduced values of plastic deformation, which can lead to an almost instantaneous destruction of the material when the ultimate load is reached.

In this regard, theoretical and practical knowledge is needed on the topological characteristics of crushed materials to reduce overtension on the surface of particles in order to obtain concrete with acceptable deformation properties, while maintaining high strength characteristics. Calculations and studies were carried out on the basis of the work of Kharhardin A.N. taking into account the scheme of levels of topological transitions of discrete systems (Fig. 1) [10–13].

Materials and Methods

Model systems are used for research: quartz sand of the Korochansky deposit (Belgorod region) and feldspar sand of the Lena river floodplain (Sakha Republic) – as microdispersed systems; nanostructured binder based on quartz sand of the Korochansky deposit (Belgorod region) and granite of the Poltava deposit (Voronezh region) are used as nano- and microdispersed systems, which composition has 10–20% of formed nanodispersed particles depending on the composition and technology of production.

The materials were crushed mechanically in a dry manner in a planetary mill for 5 hours. The preparation of the nanostructured binder was carried out by continuous milling of raw material in an aqueous medium with control of temperature and pH.

The empirical method for calculating the packing density of crushed particles is as follows: firstly, the bulk density of the material is measured. The sample of bulk material in the volume is selected at least twice the capacity of the vessel 100 cm^3. The sample is preliminarily weighed, then the vessel 100 cm^3 must be filled with material without compression under the influence of free fall up to matchmarks or edges depending on the type of vessel. Then the remainder of the sample is weighted. Bulk density and packing density are calculated by the formulas (Eq.1) and (Eq.2), respectively.

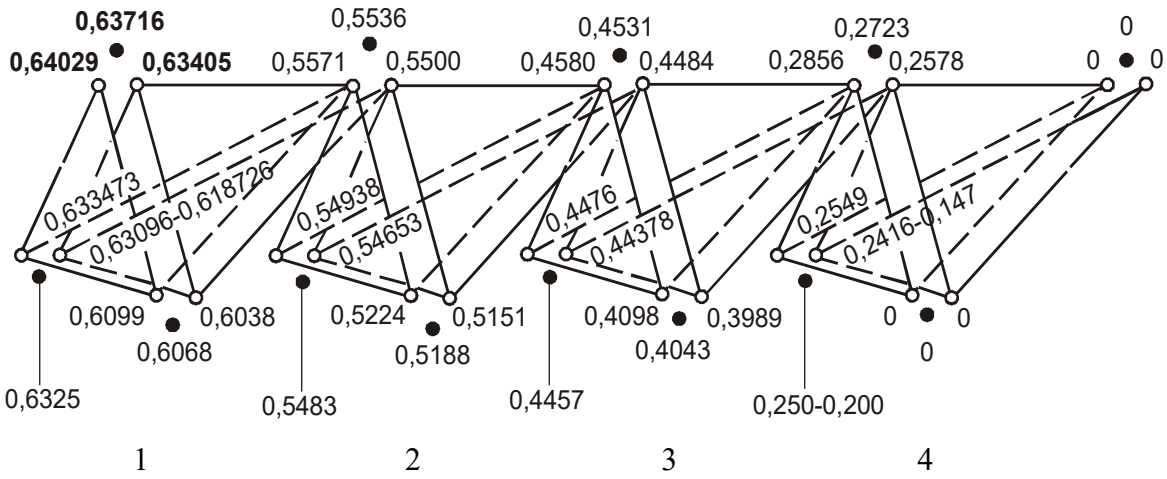

Fig. 1. The standard scheme of the main levels of the phase-topological states of disordered condensed discrete systems: 1, 2 – pseudo-solid; 3 – pseudo-liquid; 4 – critical state of the dispersed layer

$$\gamma = \frac{m_0 - \Delta m}{100}. \quad (1)$$

where m_0 – weight of the selected sample, g;
Δm – weight of the remainder of the sample, g.
The packing density of particles is calculated by the formula

$$\eta = \frac{\gamma}{\rho_м}. \quad (2)$$

where γ – calculated bulk density of the material, g/cm^3;
$\rho_м$ – true density of the material, g/cm^3.

The difference in the method for determining the packing density in an aqueous medium is the filling of the vessel with bulk material in 3 steps. The material is filled in a third, leveled, then with a dropper drop-wise water is filled, while the material absorbs water drops and it changes the initial volume of the material in the direction of decrease. Water should be added before the appearance of a water film above the material. These actions are repeated twice more up to filling the vessel to the established level of 100 cm3. Formulas for calculation are the same.

Calculations of topological characteristics were carried out using the scheme of levels of topological transitions of discrete systems on the basis of works by Kharhardin A.N. [10–13]. These include the average distance between particles of dispersed materials, characterized by the packing density and the shape factor of the particles, determined by the ratio of the surface area of non-interacting irregularly shaped particles to the surface area of spherical particles of equal volume.

Results

The density of packing of microparticles in the volume of large (2 ... 3 mm) aggregations reached the value = 0,906, and in the surface layers it corresponded to the densest packing of balls on the plane $\eta = \pi / 2\sqrt{3} = 0{,}9069$. The source and carrier of the charges of the Coulomb interaction of particles is their surface and the radius of its curvature. After drying of crushed materials at 150 °C, the packing density of their particles increased to a design value of 0,818.

Taking into account the interaction of particles through repulsion and attraction forces, the shape factor in the dispersed layer will be determined by the degree of deformation of the electrostatic shell due to sharp taper angles. At points of contact of taper angles of the particles there are attraction forces that lead to the formation of loose structures in the dispersed layer, so the packing density of the microparticles in it decreases (Table 1). Subsequent milling by dry process results in the aggregation of microparticles with size less than 3–1 μm with their packing density in a loose dispersed layer where the average value is = 0,255.

Table 1. Characteristics of mechanically activated silica-containing raw materials

Time of milling, *t,min*	Specific surface, m^2/kg	Quartz sand			+ H_2O			feldspar sand			+ H_2O		
		m, g	*γ, g/cm³*	*η*	*m, g*	*γ, g/cm³*	*η*	*m, g*	*γ, g/cm³*	*η*	*m, g*	*γ, g/cm³*	*η*
0	–	160,92	1,609	0,610	165,16	1,652	0,626	159,26	1,593	0,610	166,75	1,668	0,639
60	300–320	112,30	1,123	0,425	140,40	1,404	0,532	99,40	0,994	0,381	140,18	1,402	0,537
120	430–450	91,93	0,919	0,348	131,05	1,298	0,491	81,85	0,819	0,314	130,68	1,307	0,501
180	520–550	79,37	0,794	0,301	124,93	1,249	0,473	74,42	0,744	0,285	122,31	1,223	0,469
240	800–830	69,99	0,700	0,265	114,73	1,147	0,435	70,90	0,709	0,272	122,01	1,220	0,467
300	930–950	67,78	0,678	0,257	116,11	1,161	0,439	70,41	0,704	0,270	121,21	1,212	0,466
NB	1500–1700	64,21	0,642	0,243	102,30	1,023	0,387	62,30	0,623	0,239	99,61	0,996	0,383

According to the data obtained (Table 1), the average packing density of micro- and nanoparticles by dry mechanical milling method reaches the calculated value obtained from the equation for $p = 3$, $m = 3$ and $n = 1$, or for $n = 2$ and $d_2 = d_1$ at the time of exposure:

$$d_2 / d_1 = \left[1/10\eta_1(\sqrt{3}-1)^p\right]^{m(n-1)/3},$$

$$\eta_1 \le 1/10\left(\sqrt{3}-1\right)^3 \le 0,2549.$$

d_1, d_2, η_1 – the average size of the monodisperse fraction of the largest particles of dispersed materials before milling and after and the packing density, respectively; $p = 0; 1; 2; 3\ldots$; $p = 3$ and $m \ge 3$ – for spontaneous packing.

The coefficient of separation of microparticles with a size of 60 ... 40 μm and with a packing density in the dispersed layer $\eta_1 = 0,548\ldots0,540$ of crushed quartz sand will be:

$$\alpha^3 = \eta_1/\eta = 0,63716/(0,548\ldots0,540) = 1,16\ldots1,18.$$

$$2\delta = [(\eta_1/\eta)^{1/3} - 1]\,\psi d = [(1,16\ldots1,18)^{1/3} - 1]\,(1,16\ldots1,18)^{2/3}(40\ldots10)\ \text{mkm} = 3,4\ldots2,4\ \text{mkm}.$$

The coefficient of separation of microparticles during milling a narrow fraction of quartz sand was calculated [3] with a particle size of 0,14–0,1 mm with a packing density $\eta = 0,6038$ of its particles in a compacted dispersed layer moistened with water, where its bulk density is equal to: $\gamma = \eta_1 \cdot \rho = 0,6038 \cdot 2640$ kg/m^3 = 1594 kg/m^3, where ρ – is the true density of quartz sand . Fine fractions were separated from the suspensions by the sedimentation method. The actual separation of microparticles in the dispersed layer will be:

$$2\delta = (\alpha^3 - 1)^{1/3}\,\psi d = \{[0,64029/(0,58\ldots0,56)]^{1/3} - 1\} \cdot [0,6038/(0,58\ldots0,56)]^{2/3}$$

$$(\mathbf{60\ldots40})\ \mu\text{m} = 2\ldots1,4\ \mu\text{m}.$$

In comparison with the potential density of packing of spherical noninteracting particles, their actual separation is:

$$2\delta = (\alpha^3 - 1)^{1/3}\,\psi d = [(0,64029/(0,50\ldots0,45) - 1]^{1/3} \cdot (1,19\ldots1,27)(\mathbf{3\ldots1})\ \mu\text{m} =$$

$$0,30\ldots0,16\ \mu\text{m},$$

Taking into account the separation of particles at different levels of dispersion, when the charges on the surface of microparticles are blocked by wetting the dry dispersed layer with water, the packing density increases by one step of the phase-topological transition on the same sublevel of the PTT scheme. For example, with average values η_1:

on the main sublevel – $0,63716 \leftarrow 0,5536 \leftarrow 0,4531 \leftarrow 0,2723$,
on the middle (critical) sublevel – $0,6325 \leftarrow 0,5483 \leftarrow 0,4457 \leftarrow 0,250$,
on the sublevel of dispersed layer free-state – $0,6068 \leftarrow 0,5188 \leftarrow 0,4043 \leftarrow 0$.

Continuous milling of quartz sand by a dry method in a ball mill leads to an increase of aggregation, forces of attraction and repulsion between microparticles and the value of $\eta_{c1.} = 0,2226\ldots0,1866$. The density of spontaneous and systematic packing of microparticles in aggregations is, respectively,:

$$\eta = (0,2226\ldots0,1866)^{1/3} = 0,6066\ldots0,5714 \text{ and } \eta = (0,2226\ldots0,1866)^{0,2} = 0,740\ldots0,714.$$

In the case of mechanical destruction of aggregations, the density of the spontaneous packing of microparticles in a dispersed layer (in the volume of the vessel) under the action of repulsive forces between them will be equal to:

– in a loose bulk layer

$$(0,6066\ldots0,5714)\cdot 0,5483 = 0,3326\ldots0,3130 \text{ and } \eta_l = (0,7404\ldots0,7144)\cdot 0,5188 = 0,3841\ldots0,3708,$$

– in a layer compacted by shaking

$$\eta_l = (0,6066\ldots0,5714)\cdot 0,6038 = 0,366\ldots0,345 \text{ and } \eta_l = (0,740\ldots0,714)\cdot 0,5483 = 0,406\ldots0,392.$$

The obtained values of $\eta_l = 0,313\ldots0,406$ characterize the pseudoliquid physical state of the dispersed layer (Fig. 1), which has the property of a liquid to flow out of vertical and horizontal holes in the vessel when applying a load on the layer. Wetting with water under saturated steam conditions will block the charges on the surface of the microparticles and seal the layer up to values $\eta_l = \mathbf{0,45\ldots0,41}$.

Disintegration of microparticles in comparison with the initial value $\eta = 0,6038$ is:

$$2\delta = (\alpha^3 - 1)^{1/3} d\psi = [(0,6038/0,45\ldots0,41)^{1/3} - 1](1,22\ldots1,29)\cdot(1\ldots0,5)\ \mu\text{m} = 125\ldots83\ \text{nm}.$$

With a wet method of milling of quartz sand, the packing density of micro- and nanoparticles decreases to a value $\eta_{c2} \le 0,1$. For spontaneous packing of particles (m =3) with p = 0 and d_n/d_1 =1 we calculate $\eta_{c2} \le 0,1$. In this case, the surface structure of microparticles is destroyed with the formation of a gel. For the sol of the fractions at p = 1 and p = 2, we also have $\eta_{c2} \le 0,1366$ and $\eta_{c2} \le 0,1866$.

Disintegration of nanoparticles in silicate sol in comparison with the first critical density of their packing is:

$$2\delta = [(0,2549/0,1)^{1/3} - 1]\ (0,2549/0,1)^{2/3}\ \boldsymbol{d} = 0,366\cdot 1,866(0,5\mathbf{\ldots}0,1)\ \mu\text{m} = 341\ldots68\ \text{nm}.$$

We arbitrarily change the quantity $2\delta/d$, to find subsequent values of η_c.

For $2\delta/d = [(\eta_c/0,1)^{1/3} - 1]\psi = 0,1866$ with ψ =1 we obtain $\eta_c = 0,167$, then:

$$2\delta = [(0,167/0,1)^{1/3} - 1]\ (0,5\mathbf{\ldots0,1})\ \mu\text{m} = 187\ldots18\ \text{nm}.$$

$$2\delta = [(0,167/0,1)^{1/3} - 1]\ (0,167/0,1)^{2/3}\ (0,5\mathbf{\ldots0,1})\ \mu\text{m} = 131\ldots26,2\ \text{nm}.$$

For $2\delta/d = [(\eta_c/0,1)^{1/3} - 1]\psi = 0,1366$ with ψ =1 we obtain $\eta_c = 0,147$, then:

$$2\delta = [(0,147/0,1)^{1/3} - 1]\ (0,3\mathbf{\ldots0,1})\ \mu\text{m} = 42\ldots14\ \text{nm}.$$

$$2\delta = [(0,147/0,1)^{1/3} - 1]\ (0,147/0,1)^{2/3}\ (0,3\mathbf{\ldots0,1})\ \mu\text{m} = 53\ldots17,6\ \text{nm}$$

The density of the packing of microparticles with the blocking of charges on their surface by wetting with a 0,5% plasticizer solution (Polyplast SP-1) increases. So the compaction of a dry dispersed layer having $\eta_{c1.} = 0,255$, by wetting with a plasticizer solution, increases to $\eta_l = 0,545$, with that we have:

$$2\delta = [(0,545/0,255)^{1/3} - 1]\cdot(0,545/0,255)^{2/3}\ (5\ldots1)\ \mu\text{m} = 2,38\ \ldots0,48\ \mu\text{m}.$$

$$2\delta = [(0,64029/0,255)^{1/3} - 1]\cdot(0,545/0,255)^{2/3}\ (5\ldots1)\ \mu\text{m} = 3,0\ldots0,60\ \mu\text{m}.$$

From this data it follows that the average distance between microparticles increases as a result of growth in the total size of the microparticles together with an organic or mineral shell adsorbed on

their surface with a thickness of $\delta = 1{,}19\ldots24$ μm, which does not completely block electrical charges on their surface. When using 0,8% and 1% plasticizer solutions, the packing density of the microparticles will increase to 0,58 and 0,60, with that we obtain:

$$2\delta = [(0{,}58/0{,}255)^{1/3} - 1] \cdot (0{,}58/0{,}255)^{2/3} (5\ldots1)\ \mu m = 2{,}74\ldots0{,}55\ \mu m.$$
$$2\delta = [(0{,}60/0{,}255)^{1/3} - 1] \cdot (0{,}60/0{,}255)^{2/3} (5\ldots1)\ \mu m = 2{,}92\ldots0{,}58\ \mu m.$$

Consequently, when the surface of microparticles is wetted with a plasticizer, charges on their surface are almost completely blocked.

The dissociation of n nanoparticles, where $n \to \infty$, in silicate ashes by milling quartz sand, and $\psi = 1$ will be:

$$2\delta = [(0{,}64029/0{,}1)^{1/3} - 1] \cdot (30\ldots20)\ nm = 26\ldots17\ \mu m.$$
$$2\delta = [(0{,}64976/0{,}05)^{1/3} - 1] \cdot (20\ldots10)\ nm = 27\ldots13\ nm.$$
$$2\delta \to [(\eta_1^{1/n\to0} / \eta_{c1}^{n\to\infty})^{1/3} - 1] \cdot d^{1/n\to0} \to \infty.$$

Summary

Thus, from the results of the study, it was revealed that the packing density of the crushed particles in small aggregations is less than 0,545 / 0,7405 <0,736, in large aggregations it is no more than 0,649976, and in the surface layers of aggregations it reaches 0,9069.

Also the following patterns occurring when milling the mineral materials are revealed:

- decrease in the average distance between microparticles, which leads to an increase in their amount in the dispersed layer;
- the shape factor of the particles tends to a spherical shape;
- manifestation of electrostatic repulsive forces when the particle sizes in the dispersed layer are less than 0.5 mm;
- with complete blockage of the charge on the surface of the particles, the packing density tends to the greatest spontaneous packing of the balls 0,64029.

The obtained results can be used to optimize the compositions of cement composites and mortars of high density and strength, in order to improve deformation properties and reduce internal overetensions.

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