NATURAL LAYER SILICATE AS A MODIFIER FOR POLYMERIC NANOCOMPOSITES

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Abstract. In the building industry increasingly used for the manufacture of structural and finishing materials are silicate-containing nanocomposites, which include multi-functional modifiers, natural substances: mica, clay, zeolites, tripoli, etc. The physical basis of the implementation mechanism of the modifying effect of nano-sized particles of silicate-containing minerals in high-matrices is considered. A significant contribution to the charge state of nanoparticles in the mechanism of forming the structure of the optimal structure is shown.
Keywords: nanoparticle, dispersion, modifying action, nanocomposite, nanomodifier.

1. Introduction

In the building industry as a functional material for the manufacture for elements of different constructions (windows and doors, transport water and gas pipelines, finishing components such as baseboards, mouldings, flooring) and finishing the residential and industrial buildings and constructions used compositions based on polymeric, oligomeric and mixtures of matrix filled with components of different dispersibility, compound and mechanism of the modifying effect.

For a proper choice of a polymer composite with certain parameters of service characteristics (strength, heat-temperature resistance, wear resistance, resistance to burning, etc.) it is necessary to establish mechanisms of interaction of components, ensuring the formation of an optimal structure.

Among the most widespread types of composite materials used in the building industry are silicate-containing nanocomposites, in which as functional modifiers are used natural components - mica, clay, tripoli, zeolites.

Despite the rapidly developing scope of silicate-containing nanocomposites, many physico-chemical aspects of their formation and processing into products remain unclear. This fact hinders the process of expanding production of functional nanocomposite materials based on polymeric and oligomeric matrices

with set parameters of service characteristics. The purpose of this work was to analyze the physical aspects of modifying macromolecular compounds of nano-sized silicate-containing particles.

2. Investigation

In modelling composite systems, which consist of a binder and a filling agent, it is possible to allocate three characteristic types of substances (Fig. 1): substance of a particle (1), binder (3) and a part adjoining a binder particle (a boundary layer, 2).
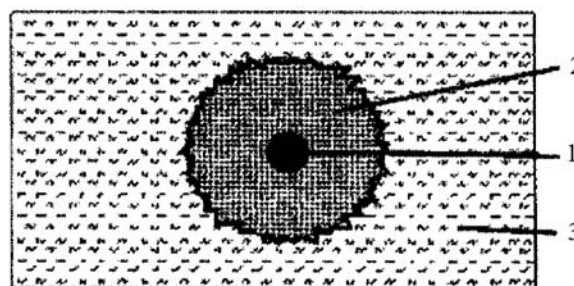

Fig. 1. Components of a modelling composite: particles filler (1), binder (3), boundary layer (2)

Let's consider the elementary case, when nanoparticles and the areas modified by them have spherical forms. Let the volume of system is equal to V, the

number nanoparticles – to N, radius of a particle – to r_j, thickness modified surface layer – to h_j.

Hence the volume of a particle is equal to

$$V_j = \frac{4}{3}\pi\, r_j^3. \tag{1}$$

Modified volume W_j is

$$W_j = \frac{4}{3}\pi\left(r_j + h_j\right). \tag{2}$$

If N – number of particles, V_j – volume of j, particles, then ratio

$$C_V = \frac{\sum\limits_{j}^{N} V_j}{V}. \tag{3}$$

Defines the relative volumes of all nanoparticles, or parking factor. The ratio

$$C_V' = \frac{\langle k \rangle \sum\limits_{j-1}^{N} V_j}{V} \tag{4}$$

represents the relative modified volume, $\langle k \rangle$ – factor of overlapping of the sites, modified by a filler particles.

3. Results

It is known from experiments that even at small concentration nanomeasure particles of the modifier (up to 0,1 mass %) the properties of a composite on the basis of polymer can essentially change. In particular for details made from a modified thermoplastic wear resistance and strength characteristics can increase by 20-30 % (Авдейчик 2007; Kittel 1956; Liopo 2003, 2005, 2007; Narai-Sabo 1969; Ouense, Pool 2). For an explanation of this experimentally fixed fact it is possible to use the following model.

Let mass concentration of particles filler C_m, mass and density filling matter m_f and ρ_f accordingly, m_b, ρ_b is the same for binder agent. Then

$$C_m = \left(1 + m_b / m_f\right)^{-1}. \tag{5}$$

From here, the volumetric concentration filler (3) is equal to:

$$C_V = \left(1 + \frac{m_b}{m_{fb}} \cdot \frac{\rho_f}{\rho}\right)^{-1}. \tag{6}$$

If the volumes (and radiuses) particles of the modifier are identical, then

$$C_V = V_1 \cdot n = \frac{4}{3}\pi\, r^3 n. \tag{7}$$

Let the thickness of the modified layer be equal to h. Then for achieving a full modifying performance of a condition the necessary condition is

$$\frac{4}{3}\pi\left(r + h\right)^3 nk = 1, \tag{8}$$

where k is the factor considering overlap and compactness of modifying areas. It follows from conditions (7) and (8):

$$\left(1 + \frac{h}{r}\right)^3 = \frac{1}{kC_V}. \tag{9}$$

As $m_b \gg m_f$, the condition (6) can be presented in the form of

$$C_V = C_m \frac{\rho_f}{\rho_b}. \tag{10}$$

Then the expression (9) will become:

$$\frac{h}{r} = \left[\frac{\rho_f}{\rho_b C_m k}\right]^{-\frac{1}{3}}. \tag{11}$$

For a limiting case when particles settle down in the points corresponding to the most dense packing of spheres with radius $(r + h)$ and an overlap is absent, k = 0,74. When $\frac{r_f}{r_b} = 4$ (typical case) and $C_b = 0,1\%$, we shall receive:

$$h \gg 15r. \tag{12}$$

Naturally, the application of the offered model is restricted, because, first, it is necessary to prove that a condition (12) takes place, and, secondly, it is necessary to consider that at the manufacture of a composite it is difficult to reach a uniform distribution of modifying particles in volume binder matter. It is shown really that according to the argotic theorem at each point of substance of a composite at its hashing fluctuation changes of density occur; and there are divergent streams that cause occurrence and disappearance structures. Thus it is possible not only a formation but also destruction of clusters.

Many lower measure particles possess their own not compensated charge with a greater time of relaxation (Avdejchik et al. 2003; Kittel 1956; Belov 1976; Gusev 2005). If the modified volume in a composite to consider as a molecular cluster, its formation around of

the charged particle of the modifier can be described as follows. The increase of the cluster's sizes occurs as a result of interaction of the polarized molecules of an environment region. From the theoretical analysis of processes of creation of a composite within the limits of various approximations the conclusion always follows that the process of developing a cluster in composite polymeric systems is inevitable. For modelling this phenomenon the use of the representations stated in (Avdejchik *et al.* 2003) is possible.

It is known (Авдейчик 2007) that electric convention in poor conduction liquids arises at action of forces on a volumetric charge of a liquid. Then considering the ionic nature of conductivity, it means that the formed charges (ions or electrons) carry away plenty of neutral molecules of a liquid. But only when the relative concentration of charges in a liquid is small ($10^{-6} \div 10^{-12}$). The mechanism of such a result is not absolutely clear. However, it is possible to offer a model of its realization. According to it, even a small size of relative concentration of charges allows to explain the movement of plenty of neutral molecules of a liquid ($10^{6} \div 10^{12}$ molecules in one charge). Neutral molecules in an electric field can be polarized and enter into interaction with a charge forming a structure "charge-layer" of dipoles. The external environment of this structure develops around itself a new layer of dipoles and so on, before some equilibrium formation which can be called "charging cluster".

The number of the molecules entering the charging cluster can be estimated by the following approximations:

1. The interaction of polarized dipole molecules of a liquid around of the central kernel is described by spherical symmetry.
2. The distribution of corners P(α) between the radius-vector which is starting with a charge, and dipole moment of a molecule submits to Gauss law with a dispersion σ.
3. The distribution of corners between dipoles of n-th and n+l-th layers are similar to distribution of corners for 1st layer.

Let's define the distribution of corners between dipoles of n-th layer and a radial direction. Let α_n is a corner between dipoles of n-th and (n-l)-th spherical layers. For the first layer distribution (α_1) looks like

$$P\left(\alpha_1\right) = \frac{1}{\left(2\pi\right)^{1/2}\sigma}\exp\left(-\frac{\alpha_1^2}{2\sigma^2}\right). \tag{13}$$

For the second layer:

$$P\left(\alpha_2\right) = \int_{-\pi}^{+\pi} P\left(\alpha_1\right)P\left(\alpha_{21}\right)d\alpha_1, \tag{14}$$

when

$$a_{21} = a_2 - a_1, \quad \sigma << \pi, \quad P\left(\alpha\right)\big|_{|\alpha|=\pi} = 0, \tag{15}$$

the expression (14) can be written down as:

$$P\left(\alpha_2\right) = \int_{-\infty}^{+\infty}\left[\frac{1}{\left(2\pi\right)^{1/2}\sigma}\right]^2 \exp\left(-\frac{\alpha_1^2}{2\sigma^2}\right)\times$$

$$\exp\left[-\frac{\left(\alpha_2-\alpha_1\right)^2}{2\sigma^2}\right]d\alpha_1 =$$

$$\frac{1}{2\pi\sigma_2}\exp\left\{-\frac{1}{2\sigma^2}\left[\left(\sqrt{2}\alpha_1 - \frac{\alpha_2}{\sqrt{2}}\right)^2 + \frac{\alpha_2^2}{\sqrt{2}}\right]d\alpha_1\right\} =$$

$$\frac{1}{2\pi\sigma^2}\exp\left(-\frac{\alpha_2^2}{4\sigma^2}\right)$$

$$\int_{-\infty}^{+\infty}\exp\left[-\frac{1}{2\sigma^2}\left(\sqrt{2}\alpha_1 - \frac{\alpha_2}{\sqrt{2}}\right)^2\right]d\alpha_1 =$$

$$\frac{1}{2\pi\sigma^2}\exp\left[-\frac{\alpha_2^2}{2\left(\sqrt{2}\sigma\right)^2}\right]\sigma\pi^{1/2} =$$

$$\frac{1}{\left(2\pi\right)^{1/2}\left(\sqrt{2}\sigma\right)}\exp\left[-\frac{\alpha_2^2}{2\left(\sqrt{2}\sigma\right)^2}\right]. \tag{16}$$

Thus, distribution of molecules dipoles corners of the second layer of environment concerning a radial direction is defined by expression:

$$P\left(\alpha_2\right) = \frac{1}{\left(2\pi\right)^{1/2}\sigma_2}\exp\left(-\frac{\alpha_2^2}{2\sigma_2^2}\right), \tag{17}$$

where $\sigma_2 = \sigma\sqrt{2}$.

Let's show, that if for (n-1)-layer fairly:

$$P\left(\alpha_{n-1}\right) = \frac{1}{\sigma_{n-1}\sqrt{2\pi}}\exp\left(-\frac{\alpha_{n-1}^2}{2\sigma_{n-1}^2}\right), \tag{18}$$

where

$$\sigma_{n-1} = \left(n-1\right)^{1/2}\sigma. \tag{19}$$

That for n-th layer fairly condition:

$$P\left(\alpha_n\right) = \frac{1}{\left(2\pi\right)^{1/2}\sigma_n}\exp\left(-\frac{\alpha_n^2}{2\sigma_n^2}\right), \tag{20}$$

where

$$\sigma_n = n^{1/2}\sigma. \tag{21}$$

Really, considering that $\alpha_{n,n-1} = \alpha_n - \alpha_{n-1}$ and $P(\alpha_n) = \int_{-\infty}^{+\infty} P(\alpha_{n-1})P(\alpha_{n,n-1})d\alpha_{n-1}$ we obtain:

$$P(\alpha_n) = \frac{1}{2\pi\sigma^2(n-1)^{1/2}} \times$$
$$\int_{-\infty}^{+\infty} \exp\left[-\frac{1}{2\sigma^2(n-1)}\right] \times$$
$$\left\{\left[\alpha n^{1/2} - \frac{\alpha_n(n-1)}{n^{1/2}}\right]^2 + \frac{\alpha_n(n-1)}{n}\right\} d\alpha_n. \tag{22}$$

Or

$$P(\alpha_n) = \frac{1}{2\pi\sigma^2(n-1)^{1/2}} \exp\left[-\frac{\alpha_n^2}{2\sigma^2 n}\right] \times$$
$$\int_{-\infty}^{+\infty} \exp\left[-\frac{[\alpha_n - \alpha_n(n-1)]^2}{2\sigma^2(n-1)n}\right] d\alpha_n. \tag{23}$$

But

$$\int_{-\infty}^{+\infty} \exp\left[-\frac{[\alpha_n - \alpha_n(n-1)]^2}{2\sigma^2(n-1)n}\right] d\alpha_n =$$
$$\frac{\sqrt{2}\sigma(n-1^{1/2})}{n^{1/2}} \cdot \pi^{1/2}. \tag{24}$$

Then

$$P(\alpha_n) = \frac{1}{2\pi^{1/2}\sigma \, n^{1/2}} \exp\left(-\frac{\alpha_n^2}{2\sigma^2 n}\right) \tag{25}$$

and

$$P(\alpha_n) = \frac{1}{(2\pi)^{1/2}\sigma_n} \exp\left(-\frac{\alpha_n^2}{2\sigma_n^2}\right), \tag{26}$$

where

$$\sigma_n = n^{1/2}\sigma. \tag{27}$$

If to accept, that the last n-layer is characterized by a dispersion of corner $\sigma_n = \pi$, then the number of molecular layers in charging cluster is defined by expression:

$$n = (\pi/\sigma)^2. \tag{28}$$

In approach of the spherical form it allows to estimate and number of molecules in the cluster (N) equals to

$$N = \frac{4\pi(nr)^3\rho}{3m}. \tag{29}$$

Where ρ is density of substance, m is mass of one molecule, r its effective radius (in the considered case it is the dipole size).

The size of the dispersion σ is defined by two opposite operating factors. The factor of the order stabilization of the polarized molecule at an electric charge is energy of communication of molecules of next two layers (u). And the factor disordering is energy of thermal movement (E). Root square the deviation of a corner α_1 from zero (σ) is defined by the ratio:

$$\sigma \approx E_T/u = kT/2u. \tag{30}$$

When calculating the energy of communication (u), it is possible to consider only axial interaction of the next molecules. It reduces u and increases σ. Thus,

$$u \geq \frac{\mu_i\mu_{1+1}}{2\pi\varepsilon\varepsilon_0 r^3}, \tag{31}$$

where μ_i is a dipole moment molecule on i-th 1ayer, r – the 1inear molecule size of contacting with surface substance, ε is a relative dielectric permeability of environment. Dipole moment of the polarized molecule of non-polar dielectric is defined by relations

$$\chi = \frac{3(\varepsilon-1)}{\varepsilon+2}, \tag{32}$$

$$\mu = \frac{\varepsilon\chi \, E}{n_0}, \tag{33}$$

where χ is polarizability of volume unit, n_0 – quantity of molecules in unit of volume, E – intensity of the electric field created by a charge.

For molecules of cluster we shall receive:

$$\mu = \frac{3(\varepsilon-1)q}{n_0(\varepsilon+2)4\pi\varepsilon \, R^2}, \tag{34}$$

where q – the central charge of cluster, R – the distance from the charge central to a molecule.

An average value of communication energy $<u>$ is defined by average value the dipole moment $<\mu>$, when $R = r/2$.

$$\langle\mu\rangle = \frac{3(\varepsilon-1)q}{\pi \, n_0\varepsilon(\varepsilon+2)r^2}. \tag{35}$$

Hence $<u>$ is defined:

$$\langle u \rangle = \frac{9(\varepsilon-1)^2 q}{2\pi^3 n_0^2 \varepsilon^3 (\varepsilon+2)\varepsilon_0 r^2}. \qquad (36)$$

Thus for σ we shall receive:

$$\sigma = \frac{kT\pi^3 n_0^2 \varepsilon^3 (\varepsilon+2)^2 \varepsilon_0 r^7}{9(\varepsilon-1)^2 q^2}. \qquad (37)$$

For poorly conduction liquids (hydrocarbonic series of type C_nH_n, C_nH_{2n}, C_nH_{2n+2} where $n = 6 \div 16$), the entering into conditions constants have values: $\varepsilon = (2\text{-}3)$, $R \approx 10\text{Å}$, $T \approx 300K$, $n_0 \approx 5 \cdot 10^{26}$ (C_8H_{16}).

Hence:

$$\sigma = \frac{1,38 \cdot 10^{-23} \cdot 300 \cdot 31 \cdot 25 \cdot 10^{52}}{9 \cdot 4 \cdot (1,96)^2 \cdot 10^{-38}}.$$

$$\frac{27 \cdot 25 \cdot 8,85 \cdot 10^{-12} \cdot 10^{-63}}{9 \cdot 4 \cdot (1,96)^2 \cdot 10^{-38}}. \qquad (38)$$

It means that we receive $\sigma \approx 0{,}15$, or $n \approx 400$. Hence, within the limits of considered model thickness of the modified layer of a polymeric matrix substance has a size of about 400 nm. In this case for full modifying all volume of polymer radius of spherical modifier particles should be equaled to about size $r > 25 \div 30$ nm. Such sizes of particles can be received in various technological ways of dispersion. At reduction of radius of particles in S time concentration of the modifier can be also reduced in S time at preservation of modifying effect. Thus, the considered model explains the action on a polymeric matrix including.

Charging clusters arise either in plasma, in gas or in a liquid, in high-molecular or other environments, but they can collapse both due to external influence and under the internal electric fields. If clusters may be simulated as a drop, and it is possible to use Rayleigh approach, according to which stability of the charged drop is defined by configuration action superficial (F_s) and Coulomb (F_c) forces:

$$F_n = 4\pi r^2 \gamma, \quad F_c = \frac{(Ze)^2}{2r}, \qquad (39)$$

where r is cluster radius, Z – number of not compensated electrons, γ – factor of a superficial tension.

At small deformations drop cluster for describing of its stability, we can take the inequality

$$Z^2 e^2 \le 16\pi\gamma r^3. \qquad (40)$$

If filling agent particles consist of spherical atoms, it is possible to apply the theory of spherical packing for describing the structure with short-range force of interaction between particles. An internal atom in such a particle is surrounded by 12 neighbouring ones forming the first coordination sphere. If it is determined, N coordination spheres and radius of the first coordination sphere to accept for unit, then the radius of N-th coordination sphere (r_N) is equal to:

$$r_N = \sqrt{N}. \qquad (41)$$

The quantity atoms (k) on N-th coordination sphere is in Table 1. It means that the most dense spherical packing as for cubic face-centered crystals. The nanoparticles after grinding of crystals may have this cell.

Table 1. Coordination numbers (k), coordination spheres (N – its number) at the most dense spherical packing with type ...ABCABC...

N	k	N	k	N	k	N	k
1	12	26	24	51	48	76	72
2	6	27	96	52	72	77	96
3	24	28	48	53	72	78	0
4	12	29	24	54	32	79	96
5	24	30	0	55	144	80	24
6	8	31	96	56	0	81	108
7	48	32	6	57	96	82	96
8	6	33	96	58	72	83	120
9	36	34	48	60	48	85	144
10	24	36	36	61	120	86	24
11	24	36	36	61	120	86	24
12	24	37	120	62	0	87	144
13	72	38	24	63	144	88	24
14	0	39	48	64	12	89	96
15	48	40	24	65	48	90	72
16	12	41	48	66	48	91	144
17	48	42	48	67	168	92	48
18	30	43	120	68	48	93	144
19	72	44	24	69	96	94	0
20	24	45	120	70	48	95	48
21	48	46	0	71	48	96	8
22	24	47	96	72	30	97	240
23	48	48	24	73	192	98	54
24	8	49	108	74	24	99	120
25	84	50	30	75	120	100	84

The quantity atoms in these particle (Q_N) is determined by formula

$$Q_N = 1 + \sum_{i=1}^{N} k_i. \qquad (42)$$

The considered models allow to understand the modifying action of doping small mass concentration nanodimensioned particles. However, for a more strict arguing adequacy of these models it is necessary for real processes to prove an opportunity of charge occurrence on surface particles. For this it is necessary to analyse the process of destruction of crystal after which there are two juvenile surfaces. These surfaces

have different energy because of defects composition etc, in crystals with their new surfaces are different. For electric charges (electrons, ions, radicals, etc.) establishment of probability of charging transition we use a barrier model (Fig. 2). There is one-dimensional dependence of potential W=W (x), where the axis x is normal to juvenile surfaces of a crystal resulted.

In Fig. 2 function W (x) looks like

$$W(x) = \begin{cases} 0, x \le 0, (I); \\ U, 0 \le x < 1, (II); \\ V, 1 \le x, (III). \end{cases} \tag{43}$$
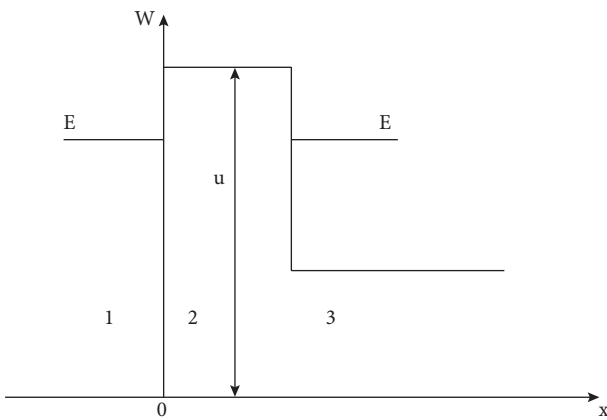

Fig. 2. A potential barrier at creation juvenile surfaces

Let's consider the movement of a particle from left to right from area 1 to 3. The wave equations for three considered areas look like:

$$\psi_j'' = k_j \psi_j = 0_{j=1,2,3}, \tag{44}$$

where

$$k_1^2 = \frac{2mE}{\hbar^2}, \quad k_2^2 = \frac{2m(E-U)}{\hbar^2},$$
$$k_3^2 = \frac{2m(E-V)}{\hbar^2}. \tag{45}$$

For the solution, we take search in the form of:

$$\psi_j = A_j \exp(ik_j x) + B_j(-ik_j x)_{j=1,2,3}. \tag{46}$$

Without breaking a generality it's possible to consider $A_1 = 1$, $B_3 = 0$ because in the field 3 there is no wave moving from right to left, if the charge moves from 1 region to the 2.

It follows from a condition of a continuity of wave function and its derivative:

$$\begin{cases} 1 + B_1 = A_2 + B_2, \\ k_1(1 - B_1) = k_2(A_2 - B_2), \\ A_2 \exp(ik_2 l) + B_2 \exp(-ik_2 l) = \\ A_3 \exp(ik_3 l), \\ k_2 A_2 \exp(ik_2 l) - k_2 B_2 \exp(-ik_2 l) = \\ k_3 A_3 \exp(ik_3 l). \end{cases} \tag{47}$$

The factor of transparency (D) barrier U to a considered case is equal:

$$D_{\rightarrow} = |A_3|^2. \tag{48}$$

A_3, as one of roots of system (48), is described by the formula:

$$A_3 = \frac{4k_1 k_2 \exp(-ik_3 l)}{(k_1 + k_2)(k_2 + k_3) \exp(-ik_2 l)} + \frac{4k_1 k_2 \exp(-ik_3 l)}{(k_1 - k_2)(k_2 - k_3) \exp(ik_2 l)}. \tag{49}$$

At the particle movement from area 3 through a barrier to area 1 at the same function W(x) (see 43), the system of the equations is:

$$\begin{cases} B_1 = A_2 + B_2, \\ k_1 B_1 = k_2(B_2 - A_2), \\ A_2 \exp(ik_2 l) + B_2 \exp(-ik_2 l) = \\ A_3 \exp(ik_3 l) + \exp(-ik_3 l), \\ k_2 A_2 \exp(ik_2 l) - k_2 B_2(-ik_2 l) \\ k_3 A_3 \exp(ik_3 l) - k_3 \exp(-ik_3 l). \end{cases} \tag{50}$$

It which follows, then:

$$B_1 = \frac{4k_2 k_3}{(k_1 + k_2)(k_2 + k_3) \exp(-ik_2 l)} + \frac{4k_2 k_3}{(k_1 - k_2)(k_2 - k_3) \exp(ik_2 l)}. \tag{51}$$

The factor of a barrier transparency at the movement of a particle from area 3 to the left is equal to:

$$D_{\leftarrow} = |B_1|^2. \tag{52}$$

Hence, the ratio of factors of a transparency is:

$$P = \frac{D_{\rightarrow}}{D_{\leftarrow}} = \frac{k_1^2}{k_3^2} = \frac{E}{E-V}. \tag{53}$$

Thus, distinction of a deficiency degree in both parties of juvenile surfaces lead to development on it electrical charge sites with the sizes of much greater atomic

power (Avdejchik *et al.* 2003, Ajayan 2004, Bragg, Claringbull 1967, Narai-Sabo 1969, Lopio 2007, Lopio 2005, Ouense, Pool 2, Lopio 2007, Gibson, Schultz 1993).

4. Conclusions

The physical basis of the implementation mechanism of the modifying effect of nano-sized particles of geosilicates in high-molecular matrices caused by the uncompensated charge with a large relaxation time is established. The presence of the charge promotes activating the adsorption interaction of polymer macromolecule with the modifier and forming in the periphery of the nanoparticle an ordered quasicrystalline layer that reinforces the composite.

Methods of forming the charge state in silicate-containing nanoparticles (thermal, mechanical, mechanochemical, etc) are determined by the composition of composite material and its functionality.

These results allow for an informed choice of components and technologies of manufacturing and processing the polymer nanocomposite materials used in the building industry.

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NATŪRALUS SILIKATAS KAIP MODIFIKATORIUS POLIMERINIAMS NANOKOMPOZITAMS

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Santrauka. Statybos pramonėje apdailos ir statybinių konstrukcijų gamybai yra plačiai naudojami nanokompozitai, kurių sudėtyje yra natūralių daugiafunkcių modifikatorių, tokių kaip molis, ceolitas, trepelis ir kt. Natūralaus silikato nanodalelėms kaip kompozito modifikatoriams įvertinti siūlomas modelis grindžiamas fizikiniais pagrindais. Straipsnyje parodytas didelis nanodalelių indėlis formuojant optimalios struktūros kompozitą atsižvelgiant į jų įkrovimo būklę.

Reikšminiai žodžiai: nanodalelė, dispersija, modifikavimas, nanokompozitai, nanomodifikatoriai.

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