Modeling the mechanical characteristics of tribotechnical composites

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Abstract. Some aspects of creating composite materials with a modified matrix based on aromatic polyamide phenylone FS-2 are considered. The effective characteristics of the composites are calculated on the basis of the self-consistency method and compared with experimental data obtained by the nanoindentation method. The stress-strain state of the composite during tribological contact was investigated on the basis of the contact problem of the motion

1. Introduction

Recently, oil-filled nanocomposites of the “oil-bearing” class have been actively used for assemblies and parts for tribotechnical applications on polymer matrices [1-3]. Obtaining a synergistic effect due to the simultaneous use of nanofillers and components with a lubricating effect, allows to achieve significant (10...25%) savings in the base material of the polymer matrix [4]. This fact significantly reduces the cost of production. Modified composite materials have a wide range of performance properties. Such materials compete with traditional metal, including ceramic, alloys. For the development of the country's economy, this increases the attractiveness of this area of materials science. In general, materials of this class can be considered as a three-component system, which consists of a polymer binder, plasticizer and multifunctional filler additives. The use of oil-filled composites in friction units requires a study of the features of contact interaction mechanics for materials of this class. In this paper, we propose one of the possible approaches to the formulation of contact problems for these materials. The theoretical basis for creating polymer composite materials that have adaptive functions in friction units is the possibility of forming adaptive principles for reducing wear and friction directly in the process of friction interaction. Theoretical approaches are based on optimizing the properties of the starting components. Moreover, the achievement of threshold values of external influence leads to a violation of the principles of compatibility of components and the formation of a certain free volume of one of the components involved in the reduction of frictional bond forces formed in the contact zone of materials. Mechanical compatibility is achieved provided that the deformation characteristics, thermal expansion coefficients, and other properties of the components correspond to each other. In this case, the integrity of the system during operation is not violated. Common to these materials is the realization of the “self-lubrication” effect
based on plasticization of polymers. It is quite obvious that the issue of creating composite oil-filled nanomaterials with adaptive operational properties requires the simultaneous consideration of a number of interrelated tasks. The solution of such problems often turns out to be contradictory, since the antifriction indices can be in conflict with the indices of the bearing ability during friction or the indices of frictional heat resistance. In this context, a plasticizer may be a substance that has pronounced lubricating properties. Such a tribological system is thermodynamically and kinetically unstable. This fact makes it possible to lay adaptive functions into it, depending on the conditions of frictional interaction at the design stage. An increase in the wear resistance of composites is achieved not only by increasing the rigidity of the polymer matrix, but also by the formation of easy slip planes in the friction transfer film due to the introduction of volumes of a lubricant with high chemical affinity for it into the polymer composition. In particular, with increasing temperature, the mobility of the macromolecular chain of the polymer matrix increases. This causes the desorption (sweating) of the plasticizer substance located in the interpackage space of the macromolecular chain outward - into the friction zone, characterized by the highest gradient of deformation and temperature. This leads to a decrease in the coefficient of friction due to a decrease in the number of physical bonds between the macromolecules of the polymer matrix and the friction surface, an increase in the flexibility and mobility of its interstitial fragments, and, correspondingly, a decrease in the temperature of the contact zone, which induces the sweating of the plasticizer. All these facts slow down the process of sweating out the substance of the plasticizer and perform the function of automatically adjusting the speed of its feed into the contact zone, equivalent to the process of wear of the polymer matrix. This means that conditions are being created for the adaptive adaptation of the composite material to friction conditions. The energy effect activates the structure of such materials, creating conditions for opening channels of energy dissipation, aimed at "healing" the resulting defects, reducing operational damage. The more intense the external energy effect is, the greater the reaction the polymer system forms, performing the function of auto-regulation of the friction characteristics of the friction unit. The use of minerals as fillers, which have the ability of metal cladding by creating a layer of inorganic polymer, as well as high absorption characteristics with respect to hydrocarbon media, the degree of which is regulated by the form of preliminary thermochemical treatment and increased dispersion (with the transition to the nanodispersed state) of minerals allows to achieve a synergistic effect of increasing antifriction characteristics of self-lubricating composites.

2. Study of the mechanical properties of composites
The authors used the aromatic polyamide phenylene FS-2 as a polymer matrix, which is designed to produce composites by injection molding. The manufacture of parts based on phenylene requires temperatures above 310-325°C. This polymer matrix is characterized by high physicomechanical properties in comparison with other polymers, which allows for the processing of parts such as grinding and polishing. The filler was magnesium aluminate spinel, ground on a NETZSCH bead laboratory mill, type MicroCer, to a size of 40-50 nm. At the stage of laboratory testing, PFMS (polymethylphenylsiloxane), VGO (non-hydrotreated vacuum gasol), bitumen, C-52 (cylinder oil) I-40 mineral oil in the amount of 5-10% were studied as plasticizer samples. Studies have established that up to external heating temperatures of 80...100°C, the coefficient of friction of oil-filled nanocomposite samples was 0.22, provided that the coefficient of friction of unmodified samples was 0.42. When the external heating temperature exceeds 100°C, the friction coefficient of the unmodified sample increased to 0.46, which led to the destruction of the sample on the friction path of 1020 m. The friction coefficient of the modified sample remained unchanged when the preheating temperature of the friction zone reached 100 °C, which confirms the structural adaptability of the material developed composite to a change in the external conditions of friction. Further determination of the mechanical characteristics of the studied composites was carried out by nanoindentation. For nanoindentation, pre-prepared samples (cylinders with a diameter of 10 mm and a thickness of 1.5 mm) from the studied materials were used. The billets were ground on a Sapphir 550 single-disk grinding and polishing machine in order to reduce the effect of the surface roughness of the test
sample on the final indentation results. The mechanical characteristics of the studied materials were determined using the NanoTest 600 complex. In this work, we considered a composite in which C-52 cylinder oil was used as a plasticizer. Oil-filled composites were molded with a ratio of components: 7% oil C-52 + 3% magnesium aluminate spinel (composition is indicated in the table). Below are the results for samples of different moldings.

| Material                        | Microhardness $H$, GPa | Elastic modulus $E$, GPa | $H/E$   | $H^3/E^2$ |
|---------------------------------|------------------------|--------------------------|---------|-----------|
| FS-2                            | 0.395                  | 5.950                    | 0.066   | 0.001741  |
| FS-2 + 3% spinel                | 0.409                  | 5.967                    | 0.069   | 0.001935  |
| FS-2 + 10% composition (v.1)    | 0.27                   | 4.931                    | 0.055   | 0.000816  |
| FS-2 + 10% composition (v.2)    | 0.255                  | 3.843                    | 0.068   | 0.001231  |
| FS-2 + 10% composition (v.3)    | 0.3                    | 4.752                    | 0.063   | 0.001219  |

As can be seen from the data in table 1, the modification of phenylone with aluminum-magnesium spinel leads to an increase in hardness and Young's modulus compared to phenylone [5]. Adding C-52 cylinder oil to the modified matrix reduces the hardness and Young's modulus, however, during tribological tests [2, 6] it was shown that the friction coefficient of such a composite material is significantly reduced (0.42..0.18) compared to phenylone.

3. Modeling the mechanical properties of composites
A very important problem when creating composite materials is the directed modeling of their effective elastic modules. In the present work, the calculation of the effective elastic constants of the composite is based on the self-consistency method. Consider an elementary representative volume of a composite medium. At each point in the medium with a radius vector $\vec{r}$ at the micro level, the generalized Hooke law:

$$\sigma(\vec{r}) = [C^m(\vec{r}) + h(\vec{r})(C^*(\vec{r}) - C^m(\vec{r}))] \cdot \varepsilon(\vec{r}),$$  \hspace{1cm} (1)

$C^m(\vec{r})$, $C^*(\vec{r})$ – tensors of elastic modules of the fourth rank of the matrix of the composite medium and inclusions, respectively, $h(\vec{r})$ – step function equal to unity inside the inclusion and zero in the matrix of a homogeneous medium. Let us average the expression (1) over an elementary representative volume under the assumption that within its limits the tensor of the elastic modules of the matrix and inclusions is constant. As a result, we obtain the following relationship:

$$\sigma(r) = C^{m}(r) \cdot \varepsilon(r) + \varphi (C^{*}(r) - C^{m}(r)) \cdot \varepsilon^{*}(r),$$  \hspace{1cm} (2)

$\varphi$ – volume fraction of inclusions, $\varepsilon^*$ – strain tensor inside inclusions. Following the ideas of [7], in the absence of interaction of inclusions, the study reduces to the problem of a single inclusion in an infinite homogeneous medium. According to this approach, expression (2) can be represented as:

$$\sigma(r) = C^{eff}(r) \cdot \varepsilon(r),$$

$$C^{eff}(r) = C^{m}(r) + \varphi (C^{*}(r) - C^{m}(r)) \cdot A(r),$$  \hspace{1cm} (3)

$$A(r) = (I + S(r) \cdot (C^{m}(r))^{-1} \cdot (C^{*}(r) - C^{m}(r)))^{-1}.$$  

$S(r)$– asymmetric Eshelby tensor [8, 9] of the fourth rank, $I$– unit tensor. The calculation of nonzero components of the elastic modulus tensor $C^{eff}$ of the composite was carried out under the assumption that the composite matrix is isotropic and the inclusions in the matrix are spherical [10].
In this case, the nonzero components of the Eshelby tensor are known and have the form [9]. It should be noted that with this form of inclusions distributed in an isotropic matrix, the desired composite inherits the isotropy of its matrix, which means that the task of determining the effective elastic moduli of the composite reduces to calculating two independent constants: \( C_{1111}^{\text{eff}}, C_{1122}^{\text{eff}} \) by which the desired values were determined \( E, \nu \). It should be noted that the considered approach to the determination of effective modules gives a result that agrees quite well with experiment only for small values of the volume fraction of inclusions (up to 15%) [11]. A series of numerical experiments was carried out to calculate the effective elastic modules of composites based on formula (3). Tables 2, 3 present the Young's modulus and Poisson's ratio for composite materials, composition 2 and 3 (table 1). In this case, for the composite composition \( v_1, v_2, v_3 \) (table 1), we first calculated the effective elastic modules of the matrix modified by magnesium aluminate spinel in a mass fraction of spinel equal to 3\% (table 2), and then the obtained values of the Young's modulus and Poisson's ratio were input data when calculating the effective elastic moduli of the desired composite depending on the volume fraction of cylinder oil (table 3). In the calculations, the following initial data were taken: Young's modulus \( E = 5.783 \) [GPa], Poisson's ratio \( \nu = 0.34 \) of the phenelone, which are determined experimentally [6], Young's modulus and Poisson's ratio of the magnesium aluminate spinel \( E = 271 \) [GPa], \( \nu = 0.26 \) [12], bulk modulus of the oil \( K = 1450 \) [Pa].

| Table 2. The dependence of the composite modules \( E, \nu \) on the volume fraction of magnesium aluminate spinel \( \varphi \). |
|-------------|-------------|-------------|
| \( \varphi \) | \( E \) (GPa) | \( \nu \) |
| 0           | 5.7830      | 0.3400      |
| 1           | 5.8982      | 0.3391      |
| 2           | 6.0132      | 0.3382      |
| 3           | 6.1283      | 0.3373      |

| Table 3. The dependence of the composite modules \( E, \nu \) on the volume fraction of oil \( \varphi \). |
|-------------|-------------|-------------|
| \( \varphi \) | \( E \) (GPa) | \( \nu \) |
| 0           | 6.1283      | 0.3373      |
| 3           | 5.7599      | 0.3316      |
| 7           | 5.2655      | 0.3222      |
| 10          | 4.8913      | 0.3130      |

Note that the obtained simulation results of effective elastic moduli of the composite were compared with the experimental data obtained on the basis of nanoindentation, given in Section 2. For example, the relative error between the experimental (table 1) and calculated Young's modulus for composite (FS-2 + 3\% spinel) did not exceed 3\%, for composite (FS-2 + 3\% spinel + 7\% cylinder oil, \( v_1 \)) did not exceed 6\%.

4. The stress-strain state of the composite material with tribological contact

In order to study the stress-strain state of a composite material under tribological contact, the contact problem of the motion of a punch with a flat base of width \( 2a \) at a speed \( V \) in the positive direction of the axis \( OX_1 \) along the boundary \( x_2 = 0 \) of an elastic isotropic half-space under the action of a force \( P = \{P_1, P_2, 0\} \) was considered. The half-space is modeled by a two-phase medium consisting of an elastic isotropic matrix and spherical inclusions, the effective modules of which are determined on the basis of the self-consistency method in Section 3. The punch moves uniformly, is in a state of ultimate equilibrium under the action of force \( P \). There is full contact with the surface of the half-space. We
assume that under the action of the normal component of the force $P$ applied to the punch with an eccentricity, only the punch settles, parallel to the axis $Ox_2$. Contact stresses are related by the Coulomb-Amonton law. The boundary of the half-plane outside the contact area is free of stresses. The method of applying external force $P$ allows us to consider the problem in a two-dimensional formulation:

$$
\begin{align*}
\sigma_{ij} &= \rho \ddot{u}_i, \quad i,j = 1,2 \\
\sigma_{ij} &= c_{ijkl} \ddot{u}_{k,l} \\
\sigma_{12} &= \sigma_{22} = 0, \quad \text{if} \quad |x_1 - Vt| > a \\
\sigma_{12} &= k \sigma_{22}, \quad \sigma_{22} = -q(x_1), \quad u_2 = -\delta, \quad \text{if} \quad |x_1 - Vt| \leq a,
\end{align*}
$$

$k$ - coefficient of friction. We assume that the speed of the punch $V$ is less than the speed of the Rayleigh wave.

Next, we move to the moving coordinate system with the origin in the center of the punch [13, 14]. Relations (4) will be considered in a moving coordinate system in a dimensionless form, with linear dimensions assigned to the half-width of the punch, and stresses to the shear modulus $G$ of the elastic matrix. It is required to determine the distribution of contact pressure $q(x_1)$ under the punch. The described problem is numerically solved by the finite element method in ANSYS. Calculation of normal and tangential contact stresses for a two-component composite material, with a matrix based on FS-2, modified with magnesium aluminate spinel (3%) and oil C-52 (7%) (table 3) was carried out for the following values: $\rho_f = 1200\ [\text{kg/m}^3]$, $\rho_m = 930\ [\text{kg/m}^3]$, speed of the punch $V/V_R = 0.1$, $V_R$ - speed of the Rayleigh wave. Based on numerical experiments, it was found that normal contact stresses are less sensitive to changes in the coefficient of friction than tangential contact stresses. The stress distribution over the contact area is asymmetric, which is typical for contact problems with friction [12], with a decrease in the coefficient of friction, the normal and tangential contact stresses decrease, the friction unit operates in a more favorable mode.

5. Conclusions
Modeling of the effective elastic moduli of the composite material gives an acceptable error, compared with the experimental data, which allows one to directionally simulate the mechanical properties of the composite. The numerical solution of the contact problem allows one to predict the friction force arising in the tribosystem when using the composite, and an increase in the content of the liquid oil fraction in the composite reduces the friction coefficient.

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