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Computing of the Molecular Orientation State of the Lubrication Layer

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Abstract

The algorithm and software for computing the order parameter value describing structural sequence in the molecular model of the boundary lubrication layer have been created. It has been shown that computer estimation of a supramolecular self-organization together with a new method of polarization tribometry can enhance the efficiency of new lubrication composition creation.

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Keywords: Lubrication materials; Lubrication layer; boundary lubrication; molecular modeling

1. Introduction

Lubrication activity of boundary layers of adsorption origin to a great extent is determined by the level of lubrication media molecules orientation in relation to friction surfaces. Currently this level is increased by introducing additions with characteristics allowing to form volume and superficial supramolecular structures (mesomorphic nanostructured systems) [1] to the lubrication media. By all means, the most important role in protecting surfaces from wear and tear is played by boundary lubrication layers, the structure of which is formed under the influence of force field of the solid surface [2, 3].

B.V. Deryagin has shown that the friction value is changed on the solid bodies surface depending on the molecules orientation in the adsorption layer. When the molecules orientation is horizontal (in relation to the base) the friction is at minimum. When the quantity of molecules of surface-active media in adsorption layer (when their

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orientation is changed from horizontal to vertical) grows the maximum friction takes place in case of their maximum disordered positions. When further the number of molecules is increased the adsorption layer acquires the most vertical orientation, the friction lessens and with further growth of the number of molecules does not change [3].

Molecular structures of boundary layer described in literature are varied and are built on the basis of general theoretical conceptions and are not likely to be verified by the experiment. However, new methods of computer molecular dynamics which have recently been developed allow researching the question of the layer structure soundly and in detail. This ideology was firstly presented by us in the work [4]. We are speaking about applying the complex of molecular modelling for describing molecular array composing the lubrication layer. Modern complexes of molecular modelling allow building adequate models of complex molecules. Examples of images of anisometric molecules able for orientation process are shown on Figure 1. THe position of each particle of this array is determined by its interaction with neighboring particles and with the solid surface. The example of modelling the interaction between the singular molecule of the mesogenic lubrication material with the metal surface (iron) is depicted on Figure 2.

In transition from the singular molecule model to the group of particles we face the necessity of the system "optimization". The essence of optimization lies in the computer software varying the position of each molecule in such a way that the system as a whole has a minimum energy. This molecular image of the lubrication layer can be subjected to pressure and/or shift. In doing that the array is deformed and each discrete step of the layer deformation is accompanied by the cyclic optimization process. The above mentioned process of supramolecular self-organization appears which is seen in the change of the molecular parameter order. The quantitative evaluation of this parameter is a real goal of the present work.

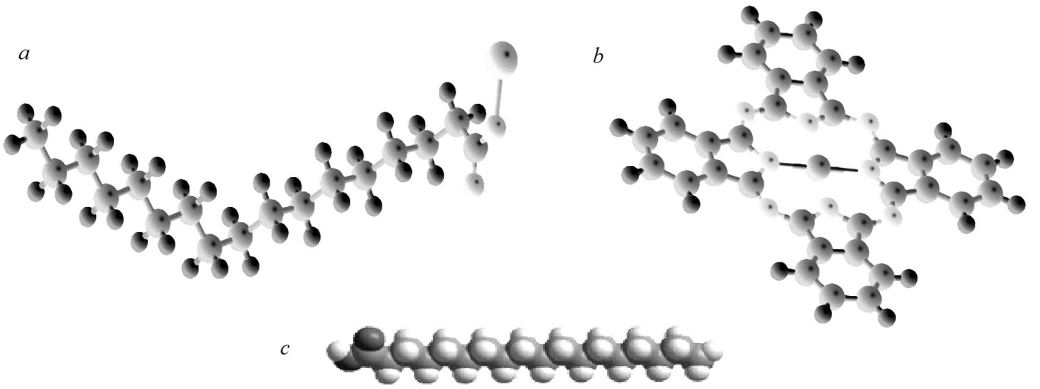

Fig. 1. Molecular models of some mesogenic molecules of tribo-active additives (*a* — sodium stearate $C_{17}H_{35}COONA$; *b* — copper phthalocyanine ($C_{32}H_{16}CuN_8$); c — oleic acid)

2. The quantitative estimation of the orientation effect in the lubrication layer with mesogenic additives

The description of orientation effects in array of molecules in the lubrication layer comes to the computing the system "order parameter". The orientation ratio can serve as one of the methods of its determination. The calculation of this ratio must be the part of a more complication calculation complex, the function of which is the molecular modelling of the friction pair with lubrication layer [5].

So, we have a group of virtual models of molecules which are moving closer to each other to create a lubrication layer in a 3-dimensional space firstly occupying random (chaotic) orientation. When imitating the friction process the shift process provides for orientating molecular axes in the direction of friction. Here appears the task of calculating the order parameter of the molecular system. This parameter must change in the process of friction depending on the structure of molecule of the triboactive component. This data can help in choosing applicable (from the point of view of tribostructuring) additions for lubrication compositions. The work [6] shows that this ratio can be calculated with the help of one of the two formulas: