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MATHEMATICAL MODEL OF BOUNDARY LUBRICATION LAYER FORMATION FROM WATER EMULSION ENVIRONMENT AT EDGE CUTTING OF METALS

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The work is devoted to the problem of efficiency of water – oil emulsions mechanical activation, applied at edge cutting of metals. It is known, that the lubricant layers, generated in conditions of limited access of external environment, have boundary mode and constructs like epitropic mesophases. But supramolecular structure and consequently tribological properties of this phase in conditions of limited access to the contact zone, strongly depend from the row of previous physicochemical processes. In the work the problem of the mathematical description of boundary lubricant layer formation process in case of edge cutting of metals in the widespread water – oil emulsional lubricooling media is solved. The fact, that preliminary dispersing of emulsions (mechano-activation), leading to decreasing of the disperse phase size, causes the essential decreasing in cutting force, has received the explanation. The description is based on the idea of microcapillary mechanism of lubrication action at edge cutting and the concept of «necessary kinetic condition for realization of lubricant action at cutting». The estimated calculations, made according to the developed model for conditions of typical mode of cutting, confirm the experimental data, received earlier. The offered formulas for calculation give the chance to predict the efficiency of mechanical emulsion lubricants activation, depending on both size distribution of small colloid particles and technological parameters of edge cutting process. It is offered to model the last stage of the process of boundary lubricant layer ordered structure formation by methods of molecular dynamics.

Key words: *lubricating process, epitropic mesophase, boundary lubricant layer, adsorption, metal cutting, emulsion, dispersing, mechano-activation, mathematical modeling.*

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МАТЕМАТИЧЕСКАЯ МОДЕЛЬ ФОРМИРОВАНИЯ ГРАНИЧНОГО СМАЗОЧНОГО СЛОЯ ИЗ ВОДОЭМУЛЬСИОННОЙ СРЕДЫ ПРИ ЛЕЗВИЙНОМ РЕЗАНИИ МЕТАЛЛОВ

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Работа посвящена проблеме эффективности механической активации водомасляных эмульсий, применяемых при лезвийном резании металлов. Известно, что смазочные слои, сформированные в условиях ограниченного доступа смазочной среды, имеют граничный характер и строятся в форме эпитропной мезофазы. Но надмолекулярная структура, а, следовательно, и трибологические свойства этой фазы в условиях ограниченного доступа, сильно зависят от предшествующих физико-химических

процессов. В работе решена задача математического описания процесса образования граничного смазочного слоя в случае лезвийного резания металлов в широко распространенных водомасляных эмульсионных смазочно-охлаждающих средах. Получил объяснение тот факт, что предварительное диспергирование эмульсий (механоактивация), приводящая к снижению размеров дисперсной фазы, вызывает существенное снижение силы резания. Описание основано на представлении о микрокапиллярном механизме смазочного действия при лезвийном резании и концепции «необходимого кинетического условия реализации смазочного действия при резании». Оценочные расчеты, выполненные согласно разработанной модели для условий типичного режима резания, подтверждают полученные ранее экспериментальные данные. Предложенные расчетные формулы дают возможность предсказывать эффективность механической активации эмульсионных смазочных материалов в зависимости от распределения размеров коллоидных частиц и режима процесса обработки. Предложено моделировать последний этап процесса формирования упорядоченной структуры граничного смазочного слоя методом молекулярной динамики.

Ключевые слова: смазочный процесс, эпитропная мезофаза, граничный смазочный слой, адсорбция, обработка металлов резанием, эмульсия, диспергирование, механоактивация, математическое моделирование.

Introduction

The lubrication process proceeding at interaction of the tool with processed material, possesses the expressed specificity caused, first of all, by limited access of environment in contact zone. In these conditions lubricant layers have small thickness, and lubrication process has a definitely boundary character. Hence, molecular orientation characteristics of the lubricant are very important for such lubricant layers.

As a rule, the adsorption-active mesogene components are present in the composition of modern metalworking fluids (MWFs). Usually these are colloid surface-active substances in the form of true or micellar solutions. But in metal working water-oil emulsions in which the surfactant plays a universal role have received the greatest application: it is both an adsorption-active film-builder and emulsifier stabilizing the emulsion. The interesting fact has been found out, that at reduction of the average size of a disperse phase in emulsion the tribological efficiency of the latter considerably increases [1]. The result of it was the offer to apply such methods of emulsion preparation which would provide decreasing of the particles size, for example, using special homogenizers [2].

Unfortunately, there is no explanation of the discovered efficiency of homogenized emulsions. In our opinion, this explanation can be found within the frameworks of the microcapillary theory of MWF's lubrication action at cutting of metals. In the present work attempt to pass from a qualitative explanation of

effect [3] to physically proved mathematical description on the basis of the processes proceeding in intersuperficial structure of microchannels has been undertaken.

The kinetic description of lubrication process

Since approximately the 80th of the last century the problem of MWF penetration kinetics into the contact zone has been solved with the microcapillary model. On section border between the tool and processed material the network of thin hollow capillaries through which lubricant penetrates is being formed. For the first time such idea was stated by M. Merchant. The first analytical models under the description of movement of the lubricant environment in an interface capillary network have been created by J. Williams and D. Tabor [4]. More profound conceptions of microcapillary lubricant process have been developed in our works [5, 6].

According to the mentioned multiphasic model, the formation of lubrication layer in case of fluent MWF goes through the following stages: 1) penetration in liquid state; 2) evaporation of liquid phase in a capillary; 3) filling of a capillary with the environment in gaseous condition; 4) formation of boundary lubrication layer as a result of adsorption and/or chemosorption; 5) formation of supramolecular structures of lubrication layer.

However, this theory has been developed for homogeneous MWF and could not take into account the dispersivity of particles in heterogeneous lubricants, such as suspensions and emulsion. It is reasonable to assume, that dispersivity – one of the

major factors influencing penetration ability of heterogeneous MWFs and, hence, on passing of described above effects at cutting of metals in multiphase environments. On the basis of the stated follows, that studying of processes of dispersing and mechano-activation of MWFs allows to create the fuller picture of lubricant action at metals cutting.

Problem statement

In the description basis lies the model represented by a single capillary. It is possible to present an individual interfacial capillary in the form of a semicylinder one end of which is closed (owing to full contact in this place between the cutting tool and chip), and the other end of it is opened to the lubrication environment (owing to the absence of such contact). Such capillary has the followuing characteristic sizes: radius r_k and length l_k. Radius r_k can limit the sizes of the disperse particles of emulsion included into the composition of MWF getting into the capillary. The presence of large particles reduces the probability of efficient filling of capillary network by tribo-active phase. Let's show how the mode of emulsion MWF penetration into capillary network essentially differs at various parities

of the size of particles d of oil phase and radius of capillary r_k.

Case 1. The emulsion contains large particles ($d >> r_k$).

Let's assume that during any moment of time the contact zone has N_k capillaries. As particles of oil phase are large, a part of capillaries will be filled exclusively by oil phase, and their remaining part – only by water (fig. 1, *a*). The proportion between these parts will correspond to the concentration of oil in water. As tribo-active component will operate only in N_k capillaries the factor of shift resistance in such capillary system will be proportional to the number of capillaries filled with oil, and it will be shown by the value of the seeming friction factor of chip movement along tool's rake face.

Case 2. Dispersed emulsion has small particles ($d << r_k$).

In this case small particles of oil, as well as water phase will necessarily get to each capillary on the interface. Since for the adsorption of organic component only a little amount of it is necessary to cover all the surface the boundary lubricant layer will be formed by the disperse phase in each capillary (fig. 1, *b*).
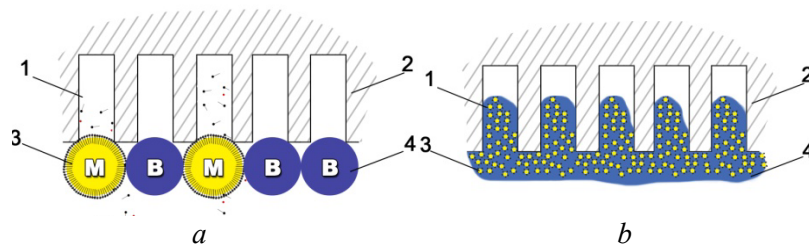

Fig. 1. The picture of emulsion MWF particles penetration into interfacial capillary network: *a* – when the diameter of a particle is more than a capillary diameter; *b* – when the diameter of a particle is less than a capillary diameter; 1 – single interfacial capillary; 2 – network of capillaries between chip and rake faces of the tool; 3 – oil disperse phase; 4 – water phase [1]

At the penetration of a water-oil lubricant into the capillary the water will intensively evaporate and push oil particles into the capillary on interphase border creating necessary tribological conditions leading to cutting force and tool wear decreasing. As we assume, besides the described above features of physical and chemical kinetics of high dispersed emulsions the possible change of their chemical compound at

mechanical activation is an important factor. As a result a destruction of spatial molecular skeleton of water takes place, as well as liberation of hydrogen bounds, formation of high reactive ions and radicals H^+ and OH^-. In the presence of oxygen, the other products possessing the oxidizing properties – hydroperoxide radical HO_2, hydrogen peroxide H_2O_2 and atomic oxygen – seem to be formed as well [7].

At water activation, radical $\dot{O}$ dissolved in water, co-operates with hydrocarbons of MWFs and oxidizes them. Depending on MWF structure, oxidation of hydrocarbons by molecular oxygen leads to formation of the big number of intermediate and final oxygen-containing products: peroxides, spirits, carbonyl substances, acids, aethers and others. Earlier it was established, that in case of oxidation of saturated hydrocarbons, presence of hydroperoxides leads to increasing of MWFs tribological activity [8]. However, within the frame of the present work we will not consider chemical aspects of formation of lubricant layer and we will be limited only to physical and physico-chemical aspects of the process.

Mathematical model

The mathematical model of lubrication action of liquid-phase MWF smears in operations of cutting materials processing should take into account at least three stages:

1. Penetration in liquid state.
2. Intensive evaporation and filling of interfacial gap by gaseous mix.
3. Formation of boundary lubrication layer, consisting from adsorbed lubricant films creating "screen" effect, leading to friction decrease.

Each of the listed above stages has indicative time of its course. As realization of lubricant action is established experimentally the *necessary kinetic condition of realization of lubricant action,* hence, is fulfilled: total time of all stages of lubrication layer formation in the capillary network cannot exceed the time of the capillary existence [6]:

$$\sum_{1}^{m} \tau_i < \tau_k \qquad (1)$$

where $\sum_{1}^{m} \tau_i$ – the sum of stages times of boundary lubricant layer formation: from penetration to supramolecular self-organizing; i – stage serial number ordered; m – number of stage; τ_k – full time of capillary existence.

Indicative time of capillary existence τ_k can be estimated under the formula [5]:

$$\tau_k = \frac{l_k}{u}, \qquad (2)$$

where u – velocity chip movement (in the order of magnitude it is equal to cutting speed V_p). At $l_k = 1$ мм

and $V_p = 0,1$ м/s we will receive average time of capillary existence: $\tau_k \sim 10^{-2}$ s.

Whence we conclude, that all the necessary processes in an individual capillary for tribological effect realization can occur during the period of time not exceeding 10 ms. As the water environment is the first to penetrate into the capillary it is this stage which defined how many contents of the disperse phase will get in contact zone. Furthermore, intensive evaporation of water pushes emulsion particles into the capillary. Then the emulsion fills in the capillary walls forming a friction reducing layer.

Let's consider the initial stage of penetration. At this stage it is important, that the size of emulsion particles would not exceed the sizes of a capillary, otherwise only the dispersive environment will get into each separate capillary. To calculate the duration of this process it is necessary to know, that time of existence of liquid phase inside the capillary mouth is defined by the indicative time of its warming up τ_p:

$$\tau_1 \approx \tau_p \sim \frac{r_k^2}{\chi} \ , \qquad (3)$$

where χ – factor of thermal diffusivity of water emulsion, which at small concentration of oil in water, is almost equal to the one of water.

Substitution of numerical values approximately corresponding to real cutting process, $\chi \sim 10^{-7} \ m^2/s$ and $r_k \sim 10^{-6} \ m$, gives the estimation of the first stage duration: $\tau_1 \approx 10^{-5}$ s. As we can see, this time is three orders less than that of the capillary existence. It is necessary to note that in this case and the duration of the liquid phase penetration into a capillary is also limited to its radius and is approximately equal to it (at the order of magnitude) because the warming up occurs in a radial direction. The estimation of the second stage duration – filling the capillary with vapor phase – was given in work [5] where the fact was stated that the speed of filling is equal in the order of magnitude of 10 m/s. Hence, the estimation of realization time of the second stage looks like:

$$\tau_2 \approx \frac{l_k}{v} \sim \frac{10^{-3}}{10} = 10^{-4} \ s \ \cdot \qquad (4)$$

From it is also can be seen that the given stage proceeds very quickly as well (the time of filling is two orders less than the time of capillary existence).

The third stage is the formation of adsorption layer. Looking at this stage it would be possible to

specify that kinetics of this layer formations is defined by huge speeds of movement of lubricant in capillary and that it practically guarantees the "shock" mechanism of such a layer formation. Thus, we can consider that almost all the organic constituent having entered into the capillary was adsorbed on its walls. Therefore, the duration of the third stage of process also ends long before the capillary closing. Hence, the necessary condition of the lubrication action realization can look as the following:

$$\tau_1 + \tau_2 + \tau_3 \leq \tau_k, \qquad (5)$$

where τ_1 – time of filling of capillary by MWF in liquid state, τ_2 – time of filling of capillary by gaseous environment, τ_3 – time of the lubricant layer formation on capillaries surfaces.

It means that the efficiency of high dispersed emulsions at cutting should be observed at higher cutting speed than at using of typical emulsions with large particles. We only need to estimate the mass of organic lubrication component of emulsion having entered into a capillary which almost fully should be adsorbed on the canal walls.

The length of a water solution penetration into the capillary l_l is approximately equal to the radius of the capillary r_k

$$l_l \sim r_k \sim 10^{-6} \, м \qquad (6)$$

The number of emulsion particles N, having entered into a cylindrical capillary, can be estimated by the equation:

$$N = c\pi r_k^2 l_l \sim c\pi r_k^3 \qquad (7)$$

where c – concentration (volumetric) of oil particles in the water environment.

Let's accept, that all particles of oil in emulsion are identical, have near spherical form and the average size d, and $\rho_м$ is the density of oil phase. Then the weight of oil component can be calculated by multiplying the particle weight by the number of such particles inside the capillary:

$$m = \rho_м \frac{\pi d^3}{6} c\pi r_k^3 = \frac{\rho_м \pi^2 r_k^3}{6} \cdot c \cdot d^3. \qquad (8)$$

Superficial density σ of emulsion oil substance on capillary walls with area $2\pi r_k l_k$ will be equal to:

$$\sigma = \frac{m}{2\pi r_k l_k} = \frac{\rho_м \pi r_k^2}{12 l_k} \cdot c \cdot d^3 = A \cdot c \cdot d^3. \qquad (9)$$

With c and d values we can operate diluting, concentrating or dispersing emulsions. Let's estimate the factor A value in this formula:

$$A = \frac{0,8 \cdot 10^3 \cdot 3,14 \cdot 10^{-12}}{12 \cdot 10^{-3}} = 0,2 \cdot 10^{-6} \sim 10^{-7} \; кг/м^2 \quad (10)$$

We will finally come to:

$$\sigma \sim 10^{-7} \cdot c \cdot d^3. \qquad (11)$$

In this formula it was assumed that the sizes and number of capillaries at edge cutting are defined by processing mode and by properties of the material processed. However, the lubricant presence can influence the distribution of stresses and deformations in the contact zone. Besides, we have found out that in case of large particles $(d \sim r_k)$, lubrication efficiency may decreases since it does not penetrate to all the areas of the contact. Therefore, the formula (11) is fair only for small sizes of emulsion particles $(d << r_k)$ and for small concentrations of oil components.

Earlier, in work [5] it was considered that the resistance to shear can be in dependence on the following factors:

$$\tau = f(N_k; c; d; r_k), \qquad (12)$$

where τ – factor of shear resistance; N_k – number of open capillaries on interphase border at fixed time; c – concentration of oil phase; d – size of particles; r_k – capillary radius.

However, the given model does not allow to define the value equal in dimension to shear stress from the values standing under the sign of function. In our opinion, the velocity of the chip movement u can be more convenient for the description of the lubricant action. Under the laws of the dimensional analysis theory, it is necessary to predict possible dependence of speed u on other values. The important thing is to register all the values included into the dependence, during the experiment. Variants of selection of the physical values included into the functional equation are based first of all on what values chip speed should depend.

The first model can be as following:

$$u = f(v, \rho, \sigma), \qquad (13)$$

where ρ – density of material processed, kg/m³; v – cutting speed, m/s; σ – surface density of tribo-active substances on capillary walls, kg/m²

In the given model the speed of cutting, density of processed material and superficial density of lubricant are used. However, the dimensional analysis of the values included into the given model allows to tell unmistakably that no dependences on the lubricant density and surface density of the lubricant can be

formed. But this statement is not supported by the experimental data. As these values play an important role in the process the model needs to be supplied with other values (or one value) which would allow to generate the complexes formed by the specified values.

We suggest adding the thermal characteristic:

$$u = f(\sigma, \rho, v, \chi) \,, \qquad (14)$$

where χ – the thermal conductivity of the lubricant m^2/s.

In this case the dimensional analysis shows that such model leads to the following parity of values:

$$u = v \cdot q\left(\frac{\sigma v}{\rho \varphi}\right), \qquad (15)$$

where $q\left(\dfrac{\sigma v}{\rho \varphi}\right)$ – a function of dimensionless complex. It is unknown and for identifying its type the experiment is needed on revealing the dependence of the chip movement speed on one of the values of this complex, for example, on cutting speed.

As soon as such dependence on any value is established we automatically receive dependences on all other values. Such system of models will be useful for practical calculations of lubrication process parameters for various lubricants and processing modes.

Conclusion

Thus, as a result of the mathematical description, presented in this work, the new explanation of the effects observed at processing of materials by cutting with application of tribo-active heterogeneous high dispersed MWFs is given. It is shown, that before the epitropic mesophase of boundary lubrication layer on interface between processed and tool materials would be made, a number of physicochemical processes should provide new formed layer by enough amount of adsorbate. The presented models give the chance to estimate expected increasing of water-oil emulsions efficiency as a result of their preliminary processing in mechanical activators (homogenizers) at a preparation stage. Beside increasing of tribological efficiency of such products their colloid stability growth is to be expected after dispersing as well. Computer molecular modeling of self-organizing monomolecular lubrication layer should be, in our opinion, the further step to development of such lubricant process complex modeling. This description will consider the mesogenic properties of MWF's organic components.

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