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Modelling of a thin soft layer on a self-lubricating ceramic composite

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Friction and wear of a self-lubricating ceramic composite under unlubricated sliding contact conditions is dependent on the formation and regeneration of a thin soft surface layer. Experimental observations have shown that a thin soft layer (third body) may be formed depending on the tribological tests conditions. This thin soft layer is a pre-requirement for the occurrence of low friction in the mild wear regime. This paper proposes a physically based model for the process of the formation and removal of the soft layer. The model is developed on the basis of mechanical stresses in the soft second phase and the elastic–plastic contact between a rough surface and a flat surface. Based on the model, the thickness of the soft surface layer on a ceramic substrate is predicted. The results show that the thickness of the soft layer is mainly determined by the mechanical properties of soft phase as well as the applied load.

1. Introduction

Self-lubricating composites are promising candidates for applications that sliding interfaces undergo in harsh conditions [1], possible applications include mechanical components experiencing high temperature conditions.

The tribological performance of the ceramic composite in contact is improved by the presence of a thin soft layer in the contact. The layer must be regenerated with time to maintain the self-lubricating ability at the interface of sliding components. Self-lubricating ceramic composites are widely used in for instance sliding bearings and cutting tool materials. According to Bowden and Tabor [2], it is well-recognized that the beneficial effect of self-lubricating composites depends on the thickness of the soft layer, the relative mechanical properties of the layer and subsurface as well as the contact pressure carried by the soft layer and substrate (first body). A few models have been introduced in literature to predict friction and wear of self-lubricating composites [3–5]. Alexeyev and Jahanmir used a slip-line field analysis to determine the process of deformation and flow of a soft phase towards the sliding interface for self-lubricating metal matrix composites [4]. Their results showed that properties of both matrix and soft second phase as well as shape and size of second phase control the soft layer formation. Bushe et al. [5] developed a model for extrusion of a soft phase on the surface of self-lubricating anti-friction aluminum alloy. In their work, the effect of the mechanical and geometric characteristics of the hard and soft phases of the aluminum alloy on the amount of the soft layer formed on the surface of the alloy in operation has been presented. Song et al. [6], developed a mechanical model to predict the thickness of a soft layer on a self-lubricating ceramic composite. They found that the thickness of the soft layer can be altered by the load and mechanical properties of the ceramic matrix and the soft second phase. In addition there are a few contact models that consider a soft film (solid lubricant) on a hard substrate and focusing on friction and wear [7–9]. However, there is no model for wear of self-lubricating composites in the current literature.

It has been observed by experiments that sliding wear of ceramics generates very fine wear particles, detached grains, deformed second phase and amorphous reaction products [10–12]. During prolonged sliding, some of these particles are ejected from the wear track and some debris remain in the wear track as shown in our earlier experimental work [11,13]. These remained debris can undergo deformation, fragmentation or chemical reaction in further sliding. The circulated debris in the contact constitute a “third body” in the sliding system and alter the contact pressure and consequently friction and wear. Valefi et al. [11,14], have recently found that a copper rich third body layer is formed during sliding tests of CuO–TZP composite against alumina and zirconia at and above 600 °C. The thickness of the third body layer is estimated by XPS analysis to be about 60 nm. Further, many experimental studies in self-lubricating composite suggested the presence of the soft layer at the sliding interface [11,15–16]. This soft layer can act as third body which reduces friction and wear [17].

Godet [18] introduced the concept of “third body” and its role on the tribological behaviour of sliding components. It is well known that the coefficient of friction is dependent on the

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properties of the third body due to velocity accommodation in the third body. Fillot et al. [19], used the third body approach to model and predict wear of two bodies in contact. In their work, an analytical analysis is proposed that considers the particle detachment process and the particle ejection process separately. However they have considered a simple qualitative model that provide formation and the removal of the third body. In order to improve the understanding of the formation and restoration of the soft layer, it is necessary to use a model which is based on the physical phenomena responsible for supply and wear of the thin soft layer [20].

The aim of this work is to develop a model for the process involved in the formation and regeneration of the thin soft layer at the surface of a ceramic composite. The outcome of the model will be discussed in the context of experiments.

2. Modelling

2.1. Mass balance of the thin soft layer

Fig. 1 represents a schematic of a rough surface in contact with a flat and smooth surface with a soft layer (third body). As described by Fillot et al. [19], the third body is fed by a “source flow” (Q_s), which is either supply by particles or material squeezed out from one of the contacting bodies; whereas particles ejected from the interface as “wear flow” (Q_w). The mass balance of the third body can be written as follows:

$$\frac{dM_i}{dt} = Q_s - Q_w \tag{1}$$

Or in thickness (time or distance dependent) as follows:

$$h_{\text{third body}} = h_{source} - h_{wear} \tag{2}$$

Based on Fig. 1 and Eq. (2), it is important for a stable thickness of the third body to have a balance between the “source flow” and the “wear flow”. The mass or thickness of this layer affects wear and if the third body layer approaches a stable thickness, the wear is more likely steady state and the composite material is protected from severe wear.

2.2. Supply to the thin soft layer

Based on this concept, it is needed to model the Q_s, so the mass flow towards the thin soft layer (third body) as well as the Q_w, being the mass flow due to wear of the thin soft layer. First, the mass flow Q_s will be addressed. Several researchers reported that a soft second phase in the self-lubricating composite can be squeezed out by contact stresses and form an interfacial layer at the interface [4,15]. For instance, Deng et al. [21] studied the self-lubricating behaviour of a Al_2O_3–TiC–CaF_2 composite under dry contact conditions. Their results indicated that the CaF_2 soft phase can be deformed and squeezed out to the interface of a sliding pair and results in the continuous formation of a tribofilm responsible for low friction and wear. Since contact stresses are imposed on a surface in contact, and the second phase is significantly softer than the matrix in a self-lubricating composite at elevated temperatures, it is reasonable to consider that the second phase can be transported to the interface by squeezing out. A mechanical model for self-lubricating ceramic composite has been recently developed. Using this model, the amount of second phase squeezed out during the sliding process can be calculated [6]. In this model, a 3D representative volume element (RVE) of the disc at the contact interface is used to analyze the formation of the transfer layer as indicated in Fig. 2 and expressed in [6]. In the analysis it is assumed that the ball and the flat are smooth, in the sense that stress concentrations due to contact at asperity level will not significantly affect the subsurface stress field. The material properties of composite are calculated using the rule of mixtures. In order to calculate the average stresses beneath a sliding point contact in the ceramic composite, the explicit equations by Hamilton [22] were used. Furthermore it is assumed that the ceramic matrix deforms elastically and the second phase undergoes plastic deformation. For simplicity, an isotropic elastic–ideally plastic second phase is considered in this model. The model of Hashin [23] for a spherical second phase in an infinite elastic matrix was used. For more details the reader is referred to [6]. The following equation has been used to calculate the thickness of squeezed out soft material layer (h_{source}) during sliding process [6]:

$$h_{source} = \alpha_{supply} \frac{1}{2b} \sum_{j=1}^{s+1} \int_0^h \int_{-b}^{b} -\psi_i \varepsilon_{sq} dydz \tag{3}$$

with

$$\varepsilon_{sq} = \begin{cases} -\varepsilon^i_{kk}(1-\theta) & \text{when} \quad \varepsilon^i_{kk} < 0 \quad \text{and} \quad \sigma^M_i = \sigma^y_i \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

in which ε_{sq} is the squeezed volume fraction of the fully dense second phase material, b and h are width and height of the RVE, σ^M_i is the equivalent von Mises stress in the second phase, Ψ is the volume concentration of the second phase and θ is the porosity of the inclusion. Therefore, flow in the inclusion will only occur in the case of hydrostatic compressive strain in the inclusion and yield of inclusion. α_{supply} is a constant related to the source flow. If all plastically deformed material is transported to the surface, then $\alpha_{supply}=1$. In reality, the second phase is deformed

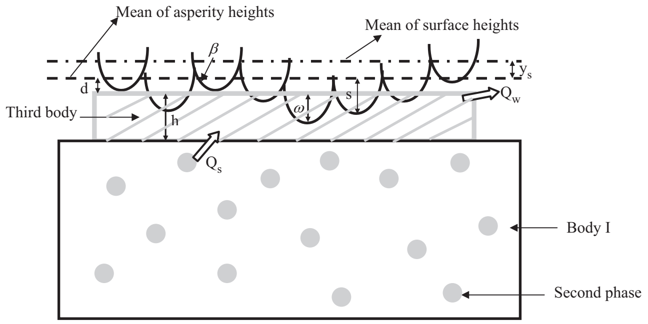

Fig. 1. Contact between a rough surface with a flat smooth surface covered with a thin soft layer (third body) generated from the self-lubricating composite.

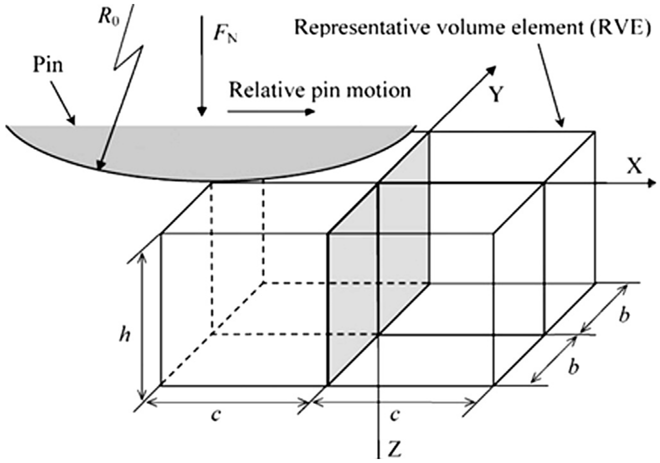

Fig. 2. Representative volume element (RVE) model for analyzing the formation of a soft layer, ball on flat configuration [6].

and transformed partially to the surface through the grain boundaries. This results in a limitation on the transport of the soft phase to the surface in the model and $\alpha_{supply} < 1$.

2.3. Wear of the thin soft layer

The soft layer (third body) is also worn away during sliding contact as shown in Fig. 1. This mass flow is denoted by Q_w. Hence, a model is required in order to calculate the wear of the third body. Liu et al. [24], investigated the effect of a deposited silver film on the wear behaviour of a steel substrate. The experimental results of their study clearly showed that plastic deformation of a soft silver film takes place due to microcutting or ploughing when a hard asperity slides through the soft film. In addition, experimental observations have shown that a soft thin film (third body) is formed on the wear track when 5CuO–TZP slides against alumina and zirconia at 600 °C [11,13–14]. The soft layer will be partly removed in time by ploughing at asperity level when the asperities of the countersurface material are penetrating the thin soft layer. Therefore the removed soft layer can transfer to countersurface material as shown in Fig. 3. The details of the experimental observation on the formation and removal of the copper rich third body layer are discussed in a previous publication [11]. Although for the supply model the situation of a smooth ball against a smooth flat is taken into account, the wear model has to take the roughness of the ploughing surface into account. Therefore, for the removal of the thin soft layer the contact will be modelled as the contact between a rough surface and a flat surface covered with a thin soft film. The resulting wear flow (Q_w) will be affected by mechanical properties and the thickness of the soft layer, the applied load as well as surface roughness of the countersurface. The mechanism for material removal is modelled on the basis of experimental observations. In the analysis, the substrate underneath the thin soft film is assumed to be elastic–plastically deforming at the length scale of contacting asperities. The soft layer (third body) is modelled as fully plastically deforming. Hence a model with a full plastic film and an elastic–plastic substrate is appropriate for the present work.

In the analysis, an asperity-based contact model is used to describe the contact behaviour [20]. The approach by Chang [7] is used to predict the amount of material removal. In this analysis, it is assumed that only the substrate is responsible for carrying the load. This assumption is reasonable due to the fact that the hardness of the soft layer is significantly lower compared to the substrate. Based on Chang's [7] model, the contact area A for a self-lubricating composite with a smooth third body can be written as follows:

$$A_{tot} = \pi\eta\beta A_n\left[\int_d^{d+\omega_c} \omega_s\phi(s)ds + \left(\frac{1}{\beta}\right)\int_d^{d+\omega_c}(a_c^2 - a_s^2)\phi(s)ds\right] + \pi\beta\eta A_n\left[\int_{d+\omega_c}^{\infty}(2\omega_s - \omega_c)\phi(s)ds + \left(\frac{1}{\beta}\right)\int_{d+\omega_c}^{\infty}(a_c^2 - a_s^2)\phi(s)ds\right] \tag{5}$$

where A_{tot} is the total contact area, η asperity density, β asperity radius, A_n nominal contact area, d separation based on asperity heights, $\phi\ (s)$ height distribution, ω_s is the substrate interference, ω_c is the critical interference at the onset of plastic deformation, a_c and a_s are the contact area radius of the third body and the substrate, respectively, see also Figs. 1 and 4.

The contact radius between the asperity and substrate can be obtained from the Hertz solution for elastic contacts and from Chang's model under elastic–plastic conditions as follows:

$$a_s = (\omega_s\beta)^{1/2} \quad \text{(Elastic contact)} \tag{6}$$

$$a_s = \left[\beta\omega_s\left(2 - \frac{\omega_c}{\omega_s}\right)\right]^{1/2} \quad \text{(Elastic–plastic contact)} \tag{7}$$

As is assumed in [7], the thin soft layer does not contribute to carrying the load, it plays a role in the size of microcontact due to low thickness and hardness of the thin soft layer. The contact area can be modelled by a load carrying central part surrounded by an annulus where the asperity is in contact with the thin soft layer. In short, the contact can be described by an inner radius a_s and an outer radius a_c.

The radius a_c is calculated as follows. It is assumed that the Hertzian stress distribution causes elastic deformation of the substrate of the flat countersurface. The deformed profile of the flat elastically-deforming countersurface can be calculated as formulated by Derjaguin et al. [25]:

$$Z(r,a_s) = \frac{1}{\pi r}\left[a_s(r^2 - a_s^2)^{1/2} - (2a_s^2 - r^2)\tan^{-1}\left(\frac{r^2}{a_s{}^2} - 1\right)^{1/2}\right] \tag{8}$$

whereas r is the distance from the center of contact area. In order to find a_c, Z is assumed to be equal to the thickness of the third body at $r = a_c$. It is assumed that the soft layer exactly follows the elastically deforming substrate. The size of the contact is determined by the fact that if the deformation is just equal to the third body thickness and $r = a_c$ is reached. This results in the implicit equation for a_c as follows [7]:

$$h_{third\ body} = \frac{1}{\pi\beta}\left[a_s(a_c^2 - a_s^2)^{1/2} - (2a_s^2 - a_c^2)\tan^{-1}\left(\frac{a_c^2}{a_s^2} - 1\right)^{1/2}\right] \tag{9}$$

It is assumed that the wear volume is the cross section area of the wear track multiplied by the sliding distance. With known values of a_c and a_s at asperity level using Eq. (9), the wear volume for an elastically-deforming asperity ploughing through a soft surface layer can be calculated. The cross section of the wear track has the shape of the difference between two spherical caps as shown in Fig. 4 (ABDE shows the removed material in Fig. 4). This results in

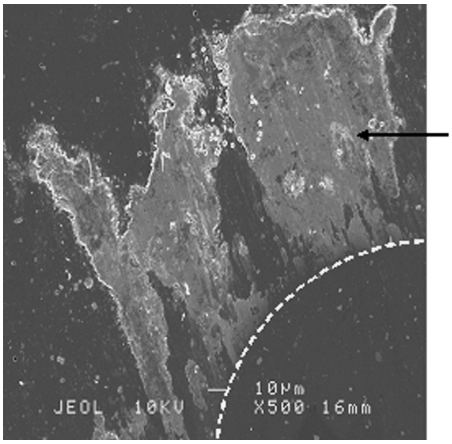

Fig. 3. Alumina countersurface sliding against 5CuO–TZP composite at 600 °C (note that the dot line indicate the contact area).

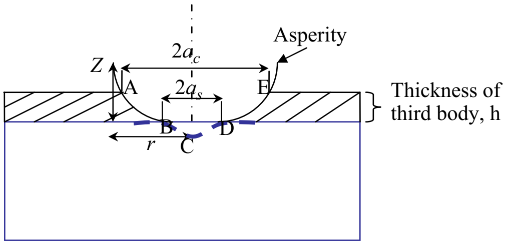

Fig. 4. Schematic representing an asperity in contact with the third body (the ABDE cap represents the removed third body).

the following expression for the wear volume:

$$h_{wear}=\frac{V_t}{A_n}=2\alpha_{wear}\eta\beta^2L\left[\int_{d-y_s}^{\infty}\left(\sin^{-1}\left(\frac{a_c}{\beta}\right)-\left(a_c\times\sqrt{(\beta^2-a_c^2)}/\beta^2\right)\right)\phi(s)ds\right.$$
$$\left.+\int_{d-y_s}^{\infty}\left(-\sin^{-1}\left(\frac{a_s}{\beta}\right)+\left(\left(a_s\times\sqrt{\beta^2-a_s^2}\right)\right)/\beta^2\right)\phi(s)ds\right] \tag{10}$$

whereas α_{wear} is the degree of wear. As it is assumed in the supply model, it is also considered that not all material is removed from the surface.

2.4. Determining α_{supply} and α_{wear}

In the model presented for the growth and removal of the soft layer α_{supply} and α_{wear} are calculated. In this section values for α_{supply} and α_{wear} are obtained based on experimental results. In order to tune α_{wear}, the obtained wear volume from experiments can be equalled to the wear volume calculated from the model. This will be further explained in below.

Fig. 5 shows a diagram that represents the different calculation steps in the model. At every X (position of ball moving against a certain plane in the disc), the source flow is used to calculate Q_s. Then the wear model is used to calculate Q_w. Finally, the resulting thickness of soft layer is calculated using Eqs. (10), (3) and (2), respectively.

In the source flow and wear model, the α_{supply} and α_{wear} are used, respectively. These two factors are determined using the specific wear rate and the thickness of the third body measured by XPS analysis as reported in our previous publication [11]. The specific wear rate measured by performing a pin-on-disc experiment is 4×10^{-7} mm^{-3}/Nm (mild wear regime). According to the experimental results, the only wear mechanism which contributes to mass loss of this soft layer is the wear flow (Q_w). This value is used to tune the α_{wear} when the k value from experiment is used.

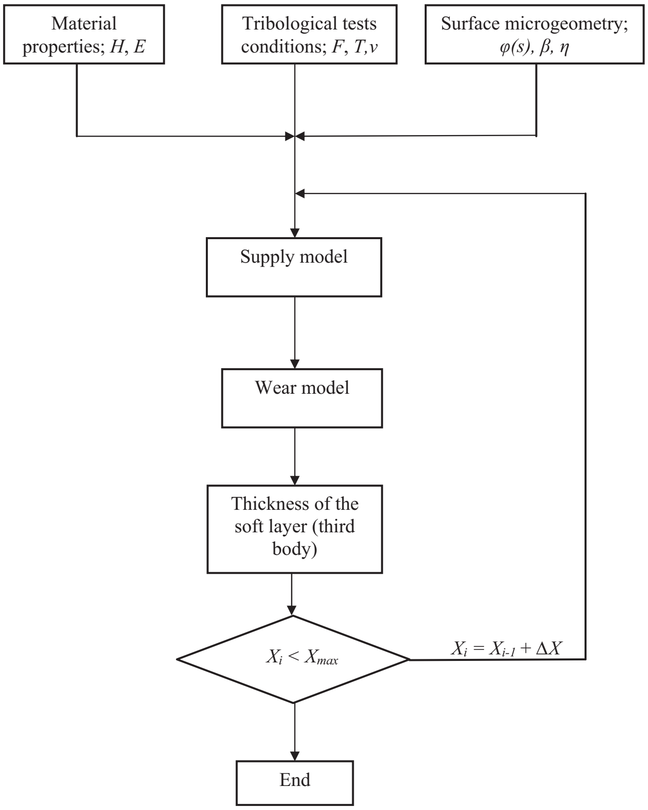

Fig. 5. Flow chart representing the soft layer formation model (X is the position of ball moving against a certain plane in the disc).

α_{wear} was varied such that the measured k value is reproduced. Given the value of the measured third body layer thickness of 60 nm and given the calculated value of α_{wear}, the α_{supply} also can be calculated by choosing α_{supply} such that the model results in the same equilibrium thickness of the layer. These two factors are used in the source flow and wear flow models.

3. Numerical results

The physical squeezing-out model and elastic–plastic contact model are used in this study to analyze the formation of the soft layer at the interface under different tribological conditions. In this section a numerical example is presented. The ball and the disc are considered to be alumina and 5 wt% CuO–TZP composite, respectively. The material properties are given in Table 1.

The hardness of the copper oxide was approximated by a value equivalent to three times of the yield stress. The geometrical parameters of the surface were obtained from a confocal image of the virgin surface (Fig. 6) to be as (see also [26]):

$$\eta=1.07\times10^{12}\ \text{m}^{-2},\quad \beta=2.77\times10^{-7}\ \text{m},\quad \sigma=1.65\times10^{-7}\ \text{m}.$$

Fig. 7 shows an example in which Q_s and Q_w are calculated for a temperature of 600 °C expressed in this case in volume flow using the density. In addition, the buildup of thin soft layer is shown for a load of 1 N and a coefficient of friction of 0.35. It is clear from Fig. 7a that Q_s increases significantly, though the Q_w increases marginally at the early stage of the contact. The system results in an equilibrium thickness of around 90 nm for a $\alpha_{supply}=2\times10^{-4}$ and $\alpha_{wear}=7.8\times10^{-2}$. This thickness value is close to the

Table 1
Material properties used for the analysis [27, 31–34].

Material properties	**Temperature (°C)**	***E* (GPa)**	***υ* (–)**	**Hardness (GPa)**	**σ_{yield} (MPa)**
CuO	500	108	0.31	0.056	20
	600	104	0.31	0.028	10
Y–TZP	500	180	0.32	5.8	2100
	600	178	0.32	4	1430
Al_2O_3	500	352	0.22	9	3200
	600	350	0.22	8.5	3030

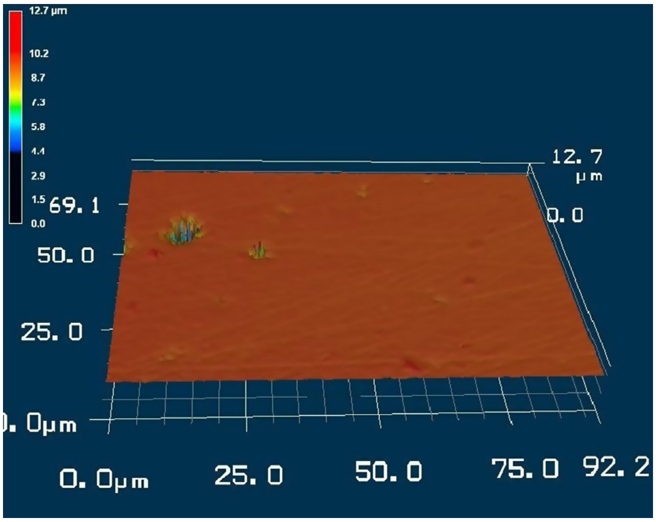

Fig. 6. 3D surface topography images of CuO–TZP disc after polishing.

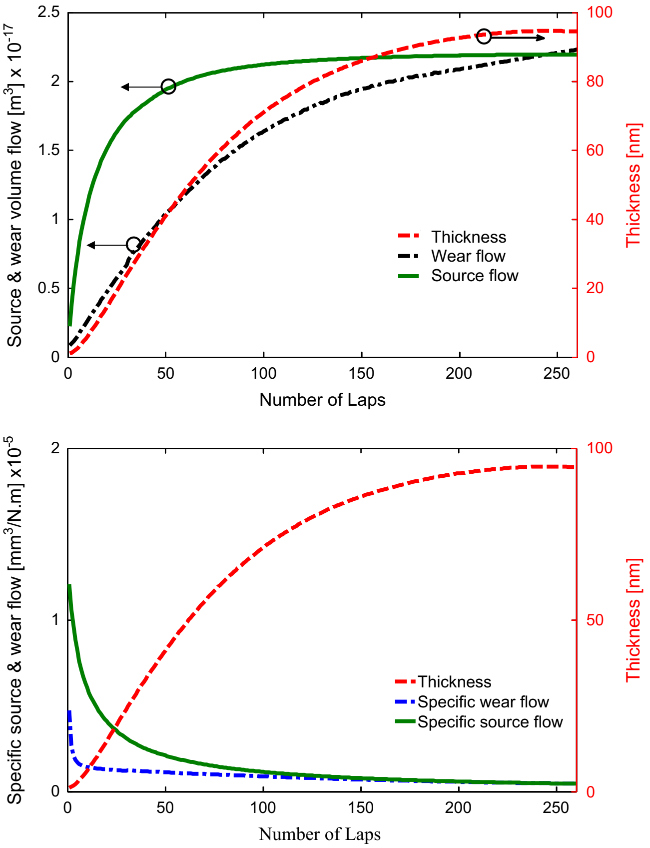

Fig. 7. (a) Source and wear volume flow as well as soft layer thickness during wear process of 5CuO–TZP sliding against alumina and (b) specific source and wear rate for the same conditions ($F=1$ N, COF=0.35, $T=600$ °C).

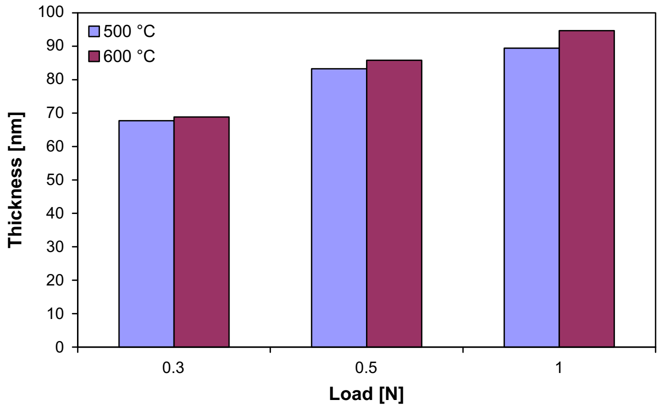

Fig. 8. Equilibrium thickness of the soft layer for different levels of temperature and applied loads after 255 sliding laps.

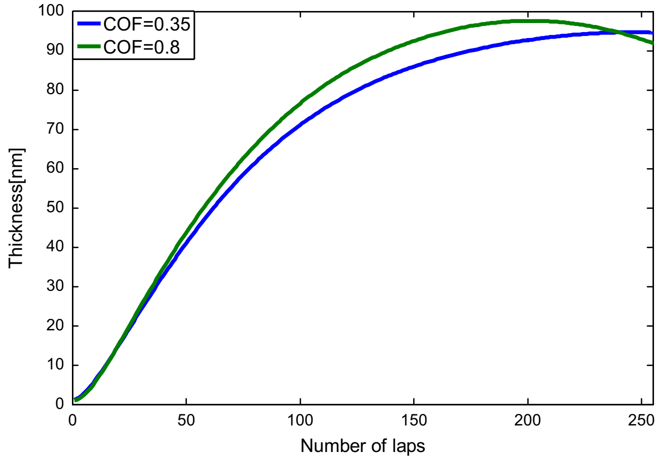

Fig. 9. Soft layer thickness development for different coefficient of friction levels.

experimentally determined thickness value [11]. In addition Fig. 7b shows that the wear rate is significant during the first laps and reaches to a steady state condition.

Fig. 8 presents the equilibrium thickness of the soft layer for different levels of temperature and applied loads using the same values for α_{supply} and α_{wear}. It is clear that at a constant temperature the thickness of the soft layer is influenced by the load. As the load increases from 0.3 N to 1 N, the equilibrium thickness of the soft third body is increased from about 70–90 nm. Furthermore, the thickness of the third body is also calculated at different temperatures. As the temperature increases at the normal load of 0.3 N the thickness of the soft layer hardly increases. However, at the normal load of 1 N the thickness of the layer increases significantly as the temperature increases. This is reasonable due to decrease in yield stress of CuO at 600 °C which influences the rate of source flow [27]. Further, Fig. 8 shows that the equilibrium soft layer thickness is influenced more by load than with temperature.

Fig. 9 shows the effect of the coefficient of friction on the thickness of the soft layer. It is obvious from this figure that coefficient of friction does not significantly influence the third body thickness. The influence of the coefficient of friction on the wear process will be further discussed in the next section.

4. Discussion

An important factor in the model is α_{supply}, representing the fraction of the plastically deforming material which ends up as part of the thin soft self-lubricating layer. In this study, α_{supply} was tuned according to the equilibrium film thickness measured using XPS for the condition of $T=600$ °C and a load of 1 N. In fact, α_{supply} is strongly dependent on the microstructure of the material. For instance, it is well known that reduction of the grain size increases the volume fraction of the grain boundaries which act as a path for the squeezing-out process [28]. This will increase the α_{supply} for composites having a smaller grain size.

In the model, it is assumed that the material, which is removed by the asperities, can partially remain in the contact. The fraction of retained material is denoted by α_{wear}. As previously mentioned, α_{wear} is estimated from experiments in this study. In reality, α_{wear} will be influenced, among others things, by the roughness of the countersurface as the asperities may operate in different wear regimes. Such effects are not taken into account in the wear model yet.

The thickness of the third body is increased as more material is squeezed out to the surface. A relatively thicker soft layer will experience more wear (Fig. 7a). For a higher normal load, a thicker soft layer is formed because the material supply due to squeezing out is higher than the material removal due to higher wear. When discussing the thickness of thin soft self-lubricating layers, it should be noted that a thicker soft layer is not necessarily better. A relatively too-thick soft layer will increase the coefficient of friction due to the decrease in load-carrying capacity of the contact. A film which has a thickness in the same order of magnitude as the surface roughness of substrate has been suggested to be effective [2,29].

As shown in Fig. 8, a higher load and higher temperature will increase the thickness of the soft layer. This is true as long as the mild to severe transition has not occurred. Based on previous publications [11,13–14], CuO–TZP shows mild wear at and below a Hertzian contact pressure of 0.52 GPa. The composition of the soft layer also plays a role in wear of the soft layer. In this model, the composition of the soft layer is assumed to be the same as the second phase in the composite. However, wear of the ceramic is caused by microfracture at the early wear stage, which will introduce debris from countersurface and disc material into the soft layer. Hence, the hardness of the soft layer could be higher than the soft phase itself due to the presence of embedded hard ceramic debris in the thin soft layer. A harder layer will enhance the load-carrying capacity. This aspect is currently neglected. If the soft layer will contribute to carrying the load, this will result in lesser wear of the substrate. However, a harder lubricating surface layer may also increase the friction level.

In the current model, μ (coefficient of friction) is an input in the source flow model. According to Fig. 9, it can be seen that μ has a minor effect on the equilibrium thickness of soft layer. It is known from previous research that the thickness of soft layer has strong influence on the μ [30]. In the case that the thickness of the soft layer has a strong influence on the μ and also if the μ has strong influence on Q_s then there would be strong feedback of the dynamic system. As can be seen from Fig. 9 this is not the case which is a positive aspect for having soft stable layer on the surface.

This study shows that a physically based model can be used to explain the thickness of the third body in a self-lubricating composite in the mild wear regime. As shown in our previous work [11], the thickness of a soft copper rich layer is experimentally estimated to be 60 nm for alumina/CuO–TZP sliding system at 600 °C and 1 N load. According to Fig. 8, the layer thickness of the third body, using the model described in this paper, is calculated to be 90 nm at $F=1$ N and 600 °C. It is, however, important to realize the limitations of the analysis. The source flow is based on the assumption of a contact for smooth surface. The analysis may not be applicable for a surface with higher roughness compared to this study. However, if the subsurface stress field is calculated e.g. by Boundary Element Method (BEM), also rough contacts can in principle be analyzed. The parameters α_{supply} and α_{wear} should be analyzed in more detail by relating these parameters to the microstructure of the ceramic composite and the microgeometry of the ploughing surface, respectively. And finally, the effect of the presence of wear debris on the hardness of the thin soft layer should be addressed. In the model, the (very thin) soft layer does not contribute to carry the load. This assumption is justified by the very small thickness and low hardness of the soft layer. Hence, a change in mechanical properties of the thin soft layer, for example by work hardening, will not influence the contact area. However, a change in the asperity radius, the thickness of the thin soft layer as well as the elastic properties of the substrate or the countersurface will influence the contact area as the contribution of the thin soft layer to the contact is solely determined by the geometrical properties of the indenting ball and the elastic contact radius on the substrate surface.

5. Conclusions

A physically based model for the formation of a thin soft layer in a self-lubricating ceramic composite during sliding process has been developed. Wear flow is modelled by ploughing on asperity level and source flow is modelled based on the squeezing-out process.

The major contributing parameters to the formation and wear of the soft layer, and therefore to the resulting thickness, are the operational conditions. It is found that the applied load has significant influence on the thickness of layer as compared to temperature for the system analyzed. Further, coefficient of friction only slightly affects the stability of system, since the coefficient of friction only has minor influence on the source flow to the thin soft layer.

Acknowledgment

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