

# About the role of tribofilms formed during automotive braking. Results of nano-scale modeling

Andrey I. Dmitriev    Werner Österle  
dmitr@ispms.tsc.ru

## Abstract

Automotive brake pads consist of many components but it is still not entirely clear which role each of the elements of this complex composition play to provide the specified regimes of sliding. Despite of the very large variety of possible brake pad formulations, the demanded performance properties are quite clear and strict: i) Stable coefficient of friction (COF) in the range 0.4-0.5 irrespective of environmental conditions, ii) wear as low as possible and iii) noise and vibration harshness (NVH). The objective of our modelling efforts was to obtain a better understanding of the sliding behaviour and associated friction properties and to study the impact of internal and external parameters on these properties. The method of movable cellular automata (MCA) was used. The third bodies were considered as aggregates of linked nanoparticles which may decompose and form a layer of granular material, the so-called mechanically mixed layer (MML), if certain fracture criteria are fulfilled. Comparison of simulation results with experimental data was done on those tests where it was possible from the side of the experimental study. The simulation results show good agreement with experimental data.

## 1 Introduction

The role of tribofilms generated during braking is discussed already about 25 years [1]. Since that time the occurrence of tribofilms was correlated either with a stabilization of the friction behaviour [2], with a decrease [1], and sometimes also with an increase [3] of friction and wear. These ambivalent interpretations are due to the fact that little was known about the structure of tribofilms formed during different braking situations and even less about structure-property relationships. Despite the permanent development of experimental methods, the area of actual contact is still difficult to access for the study directly in the test. In this regard, computer modeling can be effectively used to study the processes realized during frictional contact. The results obtained by the modeling, can form the basis of forecasting the behavior of materials rubbing on each other and provide further improvement of tribological properties.

Since 2006 the authors have started to model the sliding behaviour of tribofilms using the method of movable cellular automata (MCA) [4] with the objective to understand their functionality during braking [5, 6, 7, 8, 9]. The most important results are the following. Smooth sliding with MML formation and minimal fluctuation of COF between subsequent time steps within the desired COF range was only obtained for multiphase structures of a brittle matrix phase with soft nanoinclusions. Smooth sliding was also observed for a pure soft material contact but with low COF. Validation of the model in terms of COF evolution was obtained by comparison with model materials of exactly the same compositions obtained by ball-milling of powder blends.

This paper gives a brief overview about the previous results and shows the impact of a variety of structural parameters of tribofilm on the sliding behaviour and the evolution of the coefficient of friction (COF). In the paper the most significant results of our recent research works is presented. More detailed information is summarized in [10].

## 2 A model of a pad-disc interface

According to experimental findings the modelling setup was designed as shown schematically in Fig. 1a. Four different materials were considered in the model. Their assumed mechanical properties at room temperature, which are needed to define their stress-strain behavior, are depicted in Fig. 1b. So, the input parameters to define the mechanical properties of each material are: Young modulus, Poisson ratio, elastic limit, yield strength, fracture strength, strain at yield strength and strain at fracture.

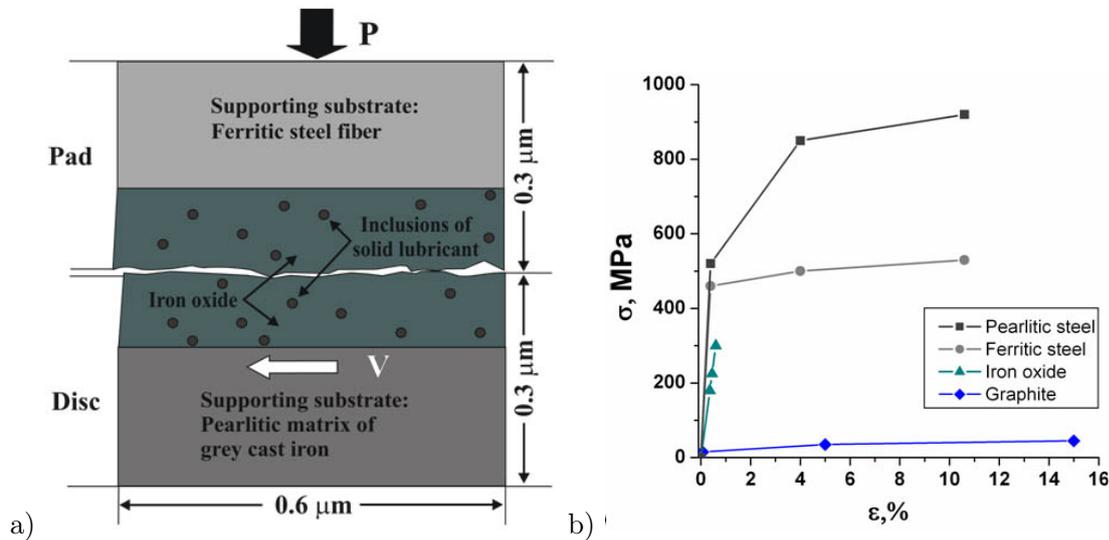


Figure 1: a) Schematic presentation of the modeled pad-disc interface b) Mechanical properties of the materials considered for MCA-modelling during previous studies (5 – 7)

The automata size, corresponding to grain size of tribofilms, was adjusted to  $10nm$  according to the smallest grain size which was experimentally determined for typical third bodies formed during automotive braking. A constant sliding velocity ( $V$ ) equal to  $10m/s$  was applied on all particles of the bottom layer of the disc. At the same time their position in vertical direction was fixed. A constant normal force corresponding to the contact pressures in the range between  $P = 15MPa$  and  $P = 50MPa$  for different calculations was acted upon all the elements of the upper layer of the pad. For both types of loading a linear procedure of value increasing was used. An initial random roughness on the nanometre scale was created artificially at both surfaces by removing some single automata from the initially flat interface. The composition of the tribofilm was kept constant at 13 vol.% soft inclusions (initially graphite as shown in Fig. 1a) embedded in iron oxide throughout this study. The time step of sliding simulation was of the order of 10 – 13s. The latter is not freely adjustable but depends on the size of automata and on their elastic properties. Periodic boundary conditions were assumed, which means that automata leaving the contact on the left side are reintroduced on the right side.

## 3 Results of modelling

### 3.1 The impact of composition. Overview of previous results

The simplest modelling setup was to assume that two steel bodies covered with nanocrystalline oxide layers, a so-called primary contact site between a steel fibre of the brake pad and the pearlitic matrix of a grey cast iron brake disc, are sliding against each other. The used model provided a reasonable mean coefficient of friction (COF) comparing well to the range desired for real braking (0.4 – 0.5) in that case. Nevertheless, friction force variations between subsequent time steps were very high and no mechanism of velocity accommodation between the moving and fixed counterparts was observed [5, 6]. This behaviour changed significantly if a certain amount of soft inclusions was added to the oxide layer.

A COF level of 0.35 was calculated for an oxide layer containing 13% graphite inclusions [7, 8, 9]. Further increase of the graphite inclusions beyond 13% did not decrease the friction level significantly [8]. A slight increase from 0.35 to 0.4 was obtained if 5% hard SiC inclusions were added to the basic model structure i.e. oxide + 13% graphite [7]. The lowest COF (0.17) was obtained with the model while assuming that the steel substrates are screened with pure graphite films and when moreover a relative high normal pressure (35MPa) was applied to an asperity contact [9]. Interestingly, the COF level was increased only slightly to 0.2, if 20% of hard SiC inclusions were added to the graphite. Obviously the COF value is dominated by the soft matrix in this case.

All simulations yielding COF-values in the range 0.17 – 0.4 correspond to smooth sliding conditions caused by MML formation and thus providing smooth velocity accommodation. Under these conditions the model predicts a pressure dependency which is correlated with MML thickness [7]. Higher friction levels can be modelled as well, but in those cases unstable friction behaviour without the mechanism of velocity accommodation within a MML is predicted.

Finally, a high and unstable COF (1.0) was modelled for a steel-on-steel contact [5, 6]. In that case compaction of particles to aggregates is quite easy, a mechanism which impedes MML formation.

In these previous studies external parameters such as temperature, mechanical properties of ingredients were kept constant while the composition of tribofilms was varied systematically. Only normal pressure was varied in a limited range in order to find conditions of optimum MML formation in respect to smooth sliding behaviour. The objective of this study was to determine the reaction of modelling results on changes of input parameters, which provides us with information about the sliding behaviour under changing external conditions. Although temperature was not directly implemented in the model, assumed changes of mechanical properties of ingredients at elevated temperatures were used to assess possible impacts of temperature on simulation results.

### 3.2 Impact of temperature-induced property changes

In the following an attempt was made for assessing possible impacts of temperature-dependent changes of mechanical properties of tribofilm constituents on modeling results. Curves  $T_1 - T_4$  of Fig. 2a are depicting possible changes of the stress-strain behaviour of the iron oxide at elevated temperatures above 800°C compared to room temperature (curve  $T_0$ ) [11]. At the moment we just wanted to find out how simulation results change if we assume that the oxide undergoes a brittle to ductile transition. Fig. 2b shows expected changes of the stress-strain behaviour of graphite at elevated temperatures. The strength of graphite increases slightly with temperature. According to available data, strength val-

ues of graphite at 1000°C amount to approximately 120% of the ones at room temperature [12]. The issue of probable impacts of a wider range of solid lubricant properties will be studied in next section.

Thus simulations were performed with the data ranges shown in Fig. 2 for the oxide and graphite, while the mechanical data of the substrate materials were kept constant. With other words, the stress-strain curves of Fig. 1b were used with modifications of the properties of the iron oxide and graphite. For the latter the curves  $T_0 - T_4$  shown in Fig. 2 were assumed successively, thus leading to curves  $T_0 - T_4$  in Fig. 3. As already shown in a previous paper, changes of the properties of substrate materials are not critical in respect to simulation results [13]. Therefore we also expect that the decrease of mechanical strength of the steel substrate at elevated temperature will not exert any impact on modeling results.

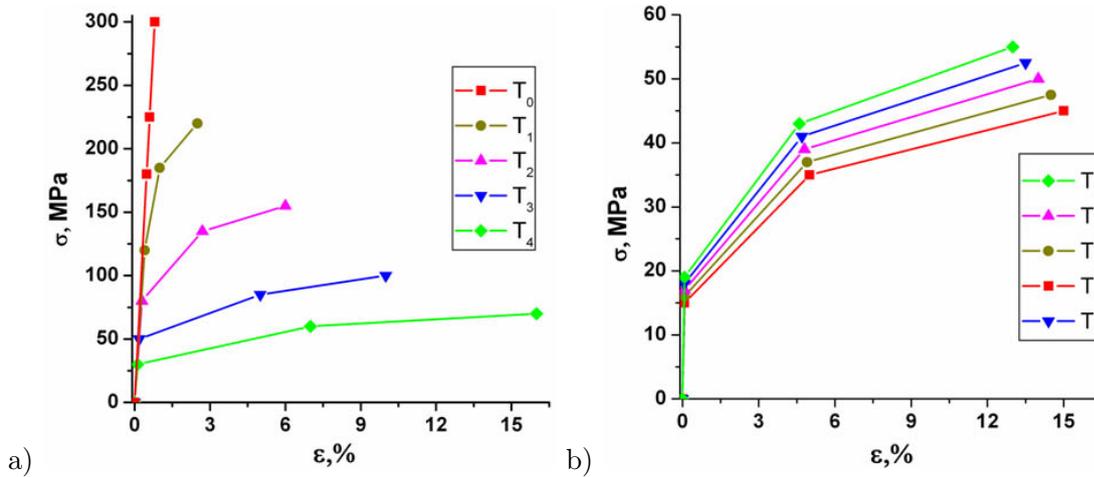


Figure 2: Modification of mechanical properties of modeled materials with respect to expected changes induced by increasing temperature,  $T_0$ : room temperature,  $T_1-4$ : elevated temperatures a) iron oxide, b) graphite

Fig. 3 shows the influence of applied pressure and changing oxide mechanical properties on the mean COF-values and the effective thickness of MML formed from the tribofilm during sliding. The layer thickness was derived from the physical coordinates of automata with missing links to their nearest neighbours. It is clearly seen that for all the cases examined COF-values decrease with increasing pressure while the MML-thickness increases. Furthermore, overall COF-levels decrease with decreasing mechanical strength of the oxide. Whereas curves  $T_1 - T_3$  look similar, there is a clear difference between  $T_0$  and  $T_4$ , especially in respect to MML-thickness variation (Fig. 3b). The observed saturation of MML-thickness at high pressure for  $T_4$  is due to the small size of the simulated set-up. In that case all automata of the tribofilms screening both first bodies are involved in the process of mixing.

The corresponding time dependencies for the calculated coefficient of friction are shown in Fig. 4. It is seen that modification of response of the model material from brittle to ductile leads not only to a reduction of the average COF values, but also to a reduction of the amplitude of COF-oscillations calculated for each time step. Both effects are most prominent when comparing conditions  $T_2$  and  $T_4$ . Thus, the smoothest sliding conditions (minimum of the amplitude of COF-oscillations) are observed in the case of the oxide showing lowest strength and highest ductility ( $T_4$ ), whilst the minimum MML-thickness is observed in the case of condition  $T_2$ .  $T_1$  and  $T_3$  show intermediate behaviour between  $T_0 - T_2$  and  $T_2 - T_4$ , respectively.

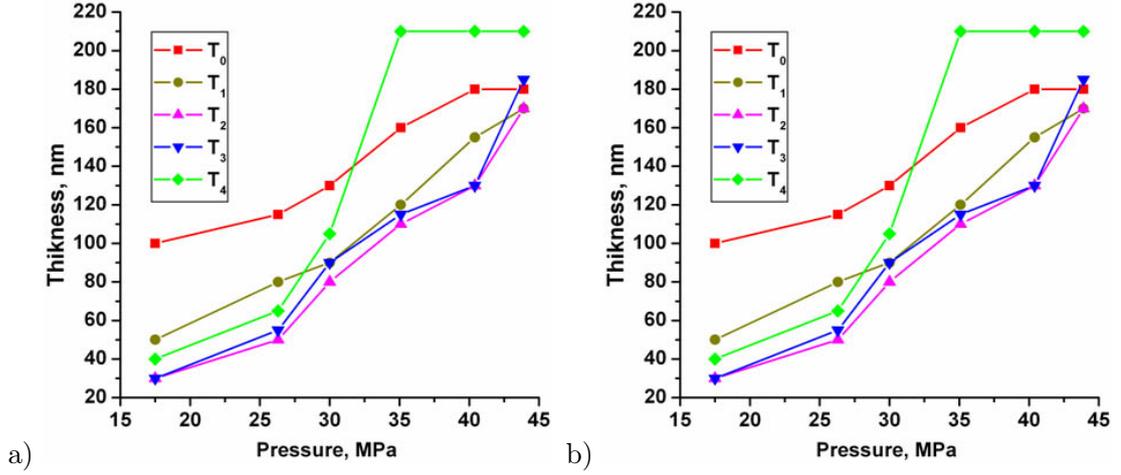


Figure 3: Modelled pressure dependencies of a) COF and b) MML thickness for various oxide properties, T0: brittle, T1-T4: ductile

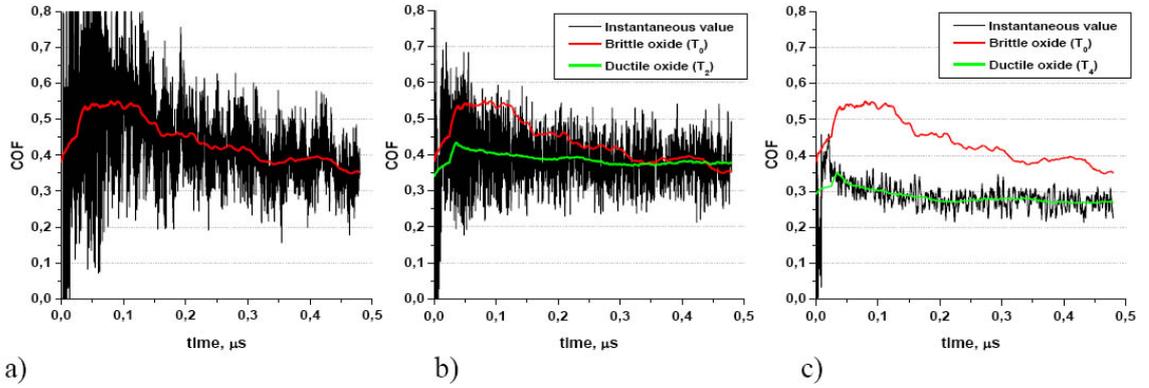


Figure 4: The time dependencies of COF for various assumed oxide properties: a)  $T_0$ , b)  $T_2$  and c)  $T_4$ . The upper curves (red in the web version) always represent mean values determined from instantaneous values of the left curve ( $T_0$ ) for comparison

### 3.3 Modification of properties of solid lubricant inclusions

In the examples shown above, expected changes of the graphite properties due to varying the temperature of the system were insignificant, only about 10% of the original values. Moreover, the shape of the response function was not changed significantly (Fig. 2b). In all of these configurations, the procedure of proportional scaling of data points on the stress - strain curve was used. However, as our previous calculations show, the particle inclusions in the friction layer are important. Under certain conditions they even may play a key role with respect to the mode of sliding of the interacting bodies. Therefore it was interesting to study the impact of different stress-strain behaviours of the soft inclusions for a wider range of properties. Such a study can help to assess the impact of different solid lubricant constituents of brake pads with respect to sliding behaviour and COF-value of tribofilms. Therefore a series of simulations was undertaken with a variation of properties of solid lubricant inclusions in the range  $-50\%$  to  $+50\%$  of the original value. The corresponding assumed response functions are shown in Fig. 5. Here the curve  $C_3$  corresponds to the original curve for graphite at room temperature ( $T_0$  in Fig. 2b). The following simulations show the impact of different solid lubricant properties embedded as nano-inclusions in

the brittle oxide film, i.e. the oxide properties correspond to  $T_0$  in Fig.2a. Note that the concentration of the particles of inclusions and their spatial distribution in the oxide matrix remained unchanged.

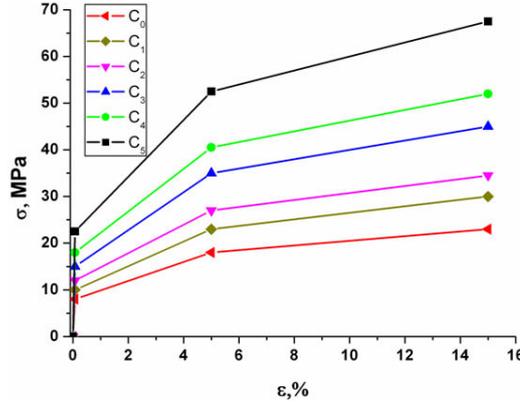


Figure 5: Modification of mechanical properties of particles of solid lubricant

The analysis of calculated time dependence of COF in the transition from the configuration with the properties  $C_0$  to  $C_5$  showed that with increasing the strength properties of inclusions an increase of the amplitude of oscillation of instantaneous values of COF obtained at each time step was also observed. It should be noted that reaching of a steady-state regime of sliding with formation of MML in the case of  $C_5$  occurs at  $2.5\mu s$  against  $1.2\mu s$  for  $C_0$ .

Similar results were obtained while assuming the same property range for the solid lubricant inclusions, but considering a ductile oxide, as characterized by curve  $T_3$  in Fig. 2a. As before, increasing the values of model parameters of the response function of the solid lubricant particles from  $C_0$  to  $C_5$  reduces the thickness of the MML. Note that the effect of reducing the MML-thickness is more pronounced compared to the brittle oxide,  $T_0$ . Thus, for the transition from  $C_0$  to  $C_5$  MML thickness is reduced about twice in this case. As before, increasing the strength properties of inclusion particles leads to an increase of the amplitude of oscillation of calculated instantaneous COF-values. Unlike the previous example, in case of the  $T_3$ -condition (ductile oxide) a steady-state regime of sliding for both cases  $C_0$  and  $C_5$  occurs within the first  $0.1\mu s$ .

Since all three parameters, namely normal pressure, property range of the oxide comprising the brittle to ductile transition, and property range of solid lubricant inclusions perform a certain impact on simulation results, it was interesting and important to assess the amount of all contributions simultaneously. This was done in terms of the steady-state COF obtained during simulations in Fig. 6. Besides normal pressure which leads to descending curves for all simulations, the brittle to ductile transition of the oxide exerts a considerable contribution as well. On the other hand, the influence of the  $\pm 50\%$  range of solid lubricant properties does not affect the general sliding behaviour very much.

## 4 Discussion and conclusions

Despite of many simplifications which had been necessary to establish the model (two-dimensional approximation, a granular structure of the modelled setup, not taken into account directly the influence of tribo-heating), the most important features for braking, namely friction force stabilization and smooth sliding conditions can be simulated quite

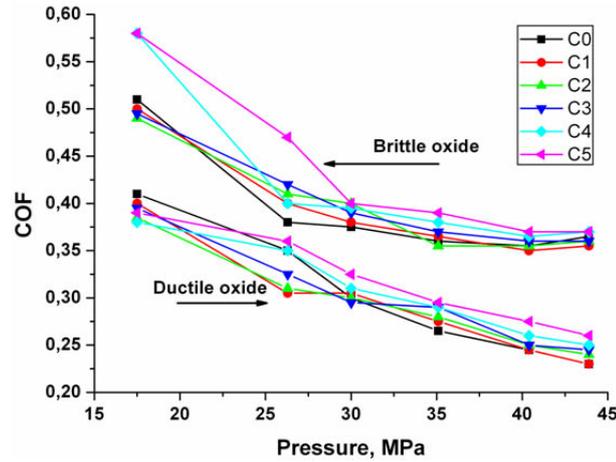


Figure 6: Pressure dependencies of COF for brittle ( $T_0$ ) and ductile oxide ( $T_4$ ) and various properties of solid lubricant particles

well provided that the friction layers show the favourable microstructure and composition which has been identified experimentally.

Based on the modelling results the following general conclusions can be drawn:

- Since smooth sliding conditions are desired for obtaining good brake performance properties, oxide films with approximately 10% of soft inclusions will usually constitute the major surface feature of brakes after a running-in period.

- Nevertheless, complete coverage of the surfaces with tribofilms without any emission of wear debris is unrealistic. Therefore, transient states will also exist locally, leading to higher friction and wear rates. Part of the wear particles will be stored in wear troughs, and this material has the potential to be spread over the surface and form a new tribofilm.

- The present study revealed that possible temperature-dependent changes of the mechanical properties of ingredients during moderate braking conditions cannot be regarded to be responsible for changes of the sliding behaviour, unless the temperature exceeds  $800^{\circ}C$ . If changes are observed experimentally, they rather will be due to changes of tribofilm composition or to its degradation. Thus an increase of COF with increasing temperature, which sometimes is observed during braking, may be due to an increased oxidation rate of the cast iron brake disc or even to elimination of tribofilms and formation of metal-on-metal contacts. For both contact situations high COF-values are predicted by the MCA-model.

- Negligible sensitivity of the simulated sliding behaviour on changing properties of the soft constituent of the tribofilm reveals that not only graphite, but any other material with mechanical properties in the range  $\pm 50\%$  of the ones of graphite will exert a similar effect.

## Acknowledgements

Financial support for this work was obtained from German Research Foundation (DFG) contract No.: OS 77/9-1, OS 77/14-1 and OS 77/19-1 and from the European Union INTAS YS-program grant 04-83-3544. Furthermore, modelling efforts were supported by the Russian Academy of Science (SB RAS), program No. III.23.2.4.

## References

- [1] Jacko M.G., Tsang P.H.S., Rhee S.K., “Wear debris compaction and friction film formation of polymer composites”, *Wear*, 133, 23-38, 1989
- [2] Chang D., Stachowiak G.V. “Review of automotive brake friction materials”, *Journal of Automotive Engineering*, 218, 953-966, 2004
- [3] Blau P.J., McLaughlin J.C. “Effects of water films and sliding speed on the frictional behaviour of truck disc brake materials”, *Tribology International*, 36, 709-715, 2003
- [4] Psakhie S.G., Shilko E.V., Smolin A.Y., et al. “Approach to simulation of deformation and fracture of hierarchically organized heterogeneous media, including contrast media”, *Physical Mesomechanics*, 14, 224-248, 2011
- [5] Österle W., Kloß H., Urban I., Dmitriev A.I. “Towards a better understanding of brake friction materials”, *Wear*, 263, 1189-1201, 2007
- [6] Dmitriev A.I., Österle W., Kloß H. “Numerical simulation of typical contact situations of brake friction materials”, *Tribology International*, 41, 1-8, 2008
- [7] Österle W., Dmitriev A.I., Kloß H. “Possible impacts of third body nanostructure on friction performance during dry sliding determined by computer simulation based on the method of movable cellular automata”, *Tribology International*, 48 128-136, 2012
- [8] Österle W., Dmitriev A.I., Orts-Gil G., Schneider T., Ren H., Sun X. “Verification of nanometre-scale modelling of tribofilm sliding behaviour”, *Tribology International*, 62, 155-162, 2013
- [9] Österle W., Dmitriev A.I., Kloß H. “Does ultra-mild wear play any role in dry friction applications, such as automotive braking?”, *Faraday Discussions* 156, 159-171, 2012
- [10] Dmitriev A.I., Österle W. “Modelling the sliding behaviour of tribofilms forming during automotive braking - impact of loading parameters and property range of constituents”, *Tribology Letters*, 53, 337-351, 2014
- [11] Hidaka Y., Anraku T., Otsuka N. “Tensile deformation of iron oxides at 600-1250°C”, *Oxidation of Metals*, 58, 469-485, 2002
- [12] European Carbon and Graphite Association (ECGA): The element C. URL link: [http://www.carbonandgraphite.org/pdf/the\\_element\\_c.pdf](http://www.carbonandgraphite.org/pdf/the_element_c.pdf)
- [13] Österle W., Kloß H., Prietzel C., Simon S., Dmitriev A.I. “On the role of copper in brake friction materials”, *Tribology International*, 43, 2317-2326, 2010.

*Andrey I. Dmitriev, Akademichesky 2/4, 634055, Tomsk, Russia*

*Werner Österle, Unter den Eichen 87, Berlin, D-12200, Germany*