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A study of third body behaviour under dry sliding conditions. Comparison of nanoscale modelling with experiment

Andrey I. Dmitriev[a], Werner Österle[b], Heinz Kloß[b] and Guillermo Orts-Gil[b]

[a] Institute of Strength Physics and Materials Science SB RAS, Akademicheskij prosp. 2/4, 634021 Tomsk, Russia; dmitr@usgroups.com
[b] Federal Institute for Materials Research and Testing (BAM), Unter den Eichen 87, Berlin D-12205, Germany

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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 plays to provide the specified regimes of sliding. This is due to the mutual interaction of multiscale mechanisms, realized during the friction. In this work we have attempted to partly answer this question using computer simulations. Since the simulation allows us to consider various combinations of the structure of the system being simulated *ceteris paribus*, it becomes possible to understand the role of each constituent sequentially. The main attention is paid to the structure and composition of the thin film that forms on the surface of both bodies as a result of compaction of the wear product, its chemical composition and oxidation. This layer, also named a third body or friction film, differs in composition and microstructure from the two first bodies. We considered a single contact for the steady state sliding when the structure and composition of friction films already are formed. As a modelling tool we used the method of movable cellular automata, which has well proven itself in solving of such tasks. We investigated the influence of modification of the structure and composition of the third body on the features of system behaviour at friction. To assess the adequacy of the numerical model, experimental studies with an artificial third body were also carried out. The simulation results are in good agreement with experimental data.

Key words: third body, dry sliding, mechanically mixed layer, computer simulation.

1. INTRODUCTION

The nature of many effects, related to friction and wear, is highly dynamic, important data about these processes can only be obtained during loading. Contact area of tribological pairs of the automotive brake pad – disk is no exception to this rule. According to observations by Godet [1], dry friction is largely determined not by the properties of friction materials of the contacting pair, but by the characteristics of the structure and composition of the thin film that forms on the surface of both bodies as a result of compaction of the wear product, its chemical composition and oxidation. This layer, also named the third body or friction film, differs in composition and microstructure from the first two bodies, which also may be modified as a result of plastic deformation. Since commercial brake pads usually are distinguished by very complicated composition and the third body is formed by compaction of the wear debris, its chemical composition usually is more complicated than the ones observed for other applications of dry friction [2]. In fact, third bodies, produced during braking, contain chemical elements from all ingredients of the pad in addition to iron oxide from the cast iron brake disc, mixed on a nanoscopic scale with grain sizes between 10 and 100 nm, depending on the type of the ingredient. The same nanostructure was observed at the surfaces of pads and discs, proving that third body films are formed on both sides by compaction of the wear debris.

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 modelling can be effectively used to study the processes, realized during the frictional contact. The results, obtained by the modelling, can form the basis of forecasting the behaviour of materials rubbing on each other and provide further improvement of tribological properties.

As long as third body films are separating the first bodies (pads and disc in the case of braking) it is quite clear that friction will be controlled by the sliding behaviour of the films rather than by properties of the first bodies. Therefore it is necessary to perform modelling on the nanoscopic scale taking into account the film thickness (approximately 100 nm) and the nanocrystalline film structure (grain size approximately 10 nm). During the friction and wear in the area of contact between the two bodies, intensive processes of deformation, generation and accumulation of damage, as well as mixing take place. Modelling of these processes can most effectively be achieved by methods that are based on a discrete approach. In this paper we use the method of movable cellular automata (MCA), which has well proven itself in solving such tasks [3–5]. Thus the purpose of this study is to investigate the influence of the structure and composition of the third body on the regime of sliding with the use of computer modelling on the basis of discrete approach.

2. THE MODEL DESCRIPTION

The MCA method is based on conventional concept of cellular automata [3]. It is an extension of cellular automaton approach, achieved by incorporating some basic postulates and relations of particle-related methods [6]. That is why the movable cellular automaton is an object of finite size, possessing translational and rotational degrees of freedom. The concept of the MCA method is based on the introduction of a new type of state, namely the state of a pair of automata. In the simplest case there are two states of the pair: linked and unlinked. The linked state is indicative of bonds between elements and the unlinked state indicates that there is no bond between automata. In the present investigations the “fracture” criteria for linked–unlinked switch was defined as critical value of stress intensity in the interacting pair *i* and *j*.

The principles of writing the equation of motion for a system of movable cellular automata and prescribing interactions between them are described in [3]. In our model, tangential forces as well as normal interaction along the line, connecting the mass centres, was used. Furthermore, the MCA method uses multiple particle interaction, which means that the force calculation is based on the spatial configuration of nearest neighbours. To express how the model works, the calculation tasks performed during a single time step are listed below. The response of each automaton during each time step was calculated in the following way. The strains and stresses of each pair of automata (which are arranged in a regular manner as described in previous papers [3–5]) are determined independently, assuming plane stress approximation [4]. The stress σ_{xx} in the specimen coordinate system is calculated [4] taking into account the influence of neighbours. Using this value, von Mises stress intensity σ_{int} is determined. After this, the criteria for linked to unlinked transition (stress intensity σ_{int} = fracture stress σ_{f}) is checked and applied accordingly. Motion of the automata mass centres is governed by the Newton–Euler equation of motion [3]. Small rearrangements of the automata continue as long as unbroken links to the neighbours exist. Only if all links are broken, larger movements become possible. After coming into contact with another automaton the unlinked–linked transition may take place. The criteria for this transition are defined as follows: 1) $\sigma = \sigma_{\text{pl}}$, $\varepsilon_{\text{pl}} = 0.2\%–0.4\%$ is an adjustable parameter for different metals; 2) $\sigma > \sigma_{\text{f}}$ is quasi-forbidden for oxides (as a rule it is not allowed, but becomes possible at special conditions); 3) forbidden for graphite; 4) forbidden for pairs of metal with oxide or graphite.

The main problem in the simulation with movable cellular automata (as, for example, by the discrete element method) is to define a particle interaction force, which provides mechanical response of a particle ensemble, conforming to simulated material or media. In our model, the experimental stress–strain curve for each considered material is used to describe mechanical properties of the corresponding automaton.

In previous papers the method MCA was used for the simulation of third body sliding [3–5,7]. The objective of modelling was to simulate mechanisms of velocity accommodation between the first bodies after a running-in period when both surfaces are screened with third body films. The nanocrystalline structure of both the films and loose wear particles, detached from the surfaces and released to the environment, suggest that the third body is an agglomerate of nanoparticles which will roll over each other if a shear stress is acting on them, but may again stick together or adhere to the substrate surface after the stress has been released.

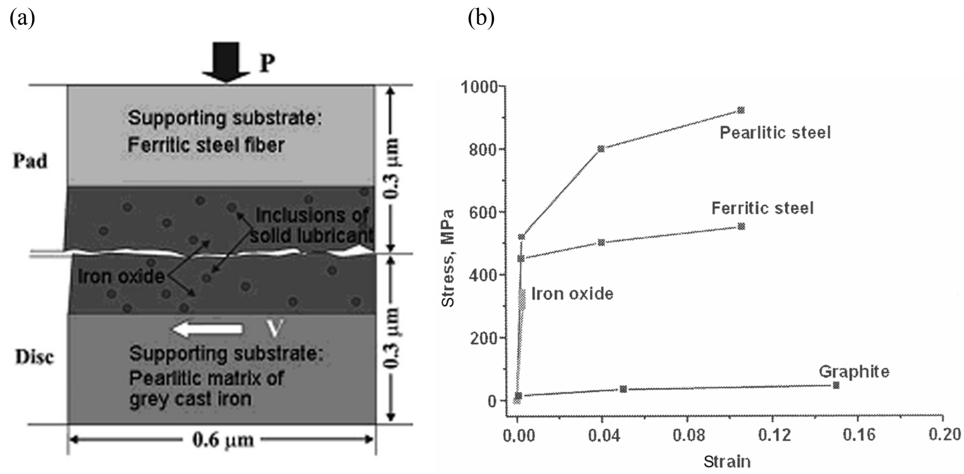

Fig. 1. (a) Schematic presentation of the modelled pad-disc interface; (b) mechanical properties of some materials considered for MCA-modelling.

According to these assumptions, the modelling set-up was designed as follows. As shown schematically in Fig. 1a, four different materials were considered in the model. The assumed mechanical properties of these four materials, which are needed to define the stress–strain behaviour, 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, ultimate tensile strength, strain at yield strength and breaking strain.

The automata size, corresponding to particle size, was adjusted to 10 nm according to the smallest grain size, which was experimentally determined for typical third bodies formed during automotive braking. A constant sliding velocity, equal to 10 m/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 *P*, corresponding to the contact pressures in the range between 15 and 50 MPa for different calculations, was applied upon all the elements of the upper layer of the pad. For both types of loading, a linear gradient was used.

3. RESULTS OF MODELLING

3.1. Requested conditions for smooth sliding

Results of our previous investigations show that to get a smooth sliding behaviour at the interface between the two first bodies it is necessary to provide conditions of a mechanically mixed layer (MML) formation [4,5,7]. According to modelling, a certain amount of soft inclusions within a rather soft but brittle oxide, like magnetite, is essential for achieving the desired properties. Neither metal-on-metal contacts nor oxide-on-oxide contacts provide stable friction conditions and a coefficient of friction (COF) around 0.4, which is desired for braking. It has been shown that a volume fraction of at least 10 vol% of soft nanoparticles (graphite in this case) is needed to form a MML, irrespective of the applied pressure. Increasing the volume fraction of soft inclusions leads to a decrease of the COF. If only 5.5 vol% soft nanoinclusions are added, the granular layer, responsible for smooth sliding behaviour, was not formed. For braking we need to accomplish two conditions: smooth sliding, but a COF as high as possible. According to our model, the fraction of soft particles should not be increased much beyond 10 vol%. A value of 13 vol% has proved to provide both, smooth sliding (sliding without big oscillation of COF) and acceptable value of the friction coefficient. The model also allows for the calculation of COF values during each time step. Results show that the mean COF at steady state sliding has dropped from 0.6 for the oxide to 0.35 for the oxide mixed with graphite.

3.2. The effect of the granulated structure

All studies presented above were based on the assumption that the outermost surfaces of both first bodies are covered by a compact and well-adhering third body film. Despite of the fact that it is not understood up to now how this film may form, there is evidence that it may be not as stable as expected, but rather may be prone to decompose as soon as normal pressure is released. Colleagues from Uppsala have observed wear debris flowing in the "labyrinth" between contact plateaus and they also found evidence for the spreading of a film at contacting sites [8]. In the meantime, several studies have proven that dust particles, emitted from brakes, show the same nanostructure as third body films [9,10]. Thus it is interesting to consider how loose wear debris, flowing in the gap between the pad and disc, may contribute to friction and sliding behaviour of the brake. A first step in this direction was undertaken with a slight modification of the MCA modelling set-up, as shown in Fig. 2a. Links between automata were broken arbitrarily along lines, thus creating a layer of loosely packed agglomerates, resembling a layer of wear debris in the gap between the first bodies. The simplest nanostructure known to provide smooth sliding conditions (iron oxide + 13% graphite) was chosen.

Figure 2b shows that also under these conditions a MML was formed during the simulation. Thus it became obvious that a layer of loose wear debris may have the same effect as a compact friction film with the same nanostructure. The difference in COF evolution for compacted and granulated structures can be observed in Fig. 3. According to the results of modelling, the set-up with granulated structure reaches smooth sliding regime faster than the similar set-up with compacted structure. Nevertheless, there is no big difference in the final mean value of COF for both considered cases.

In conclusion it can be stated that the third body films and loose wear debris, which usually cover pad and disc surfaces during automotive braking, may readily form very thin quasi-fluid layers. Such layers can account for velocity accommodation between the rotating brake disc and the fixed pad and thus are an important prerequisite for smooth sliding conditions.

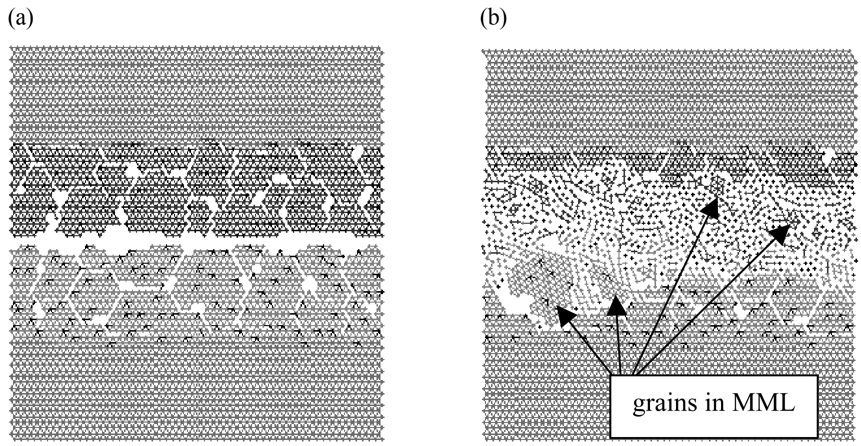

Fig. 2. Modelling set-up for a third body (13% graphite, P = 30 MPa) consisting of loosely packed agglomerates (wear debris): (a) initial configuration; (b) after sliding simulations.

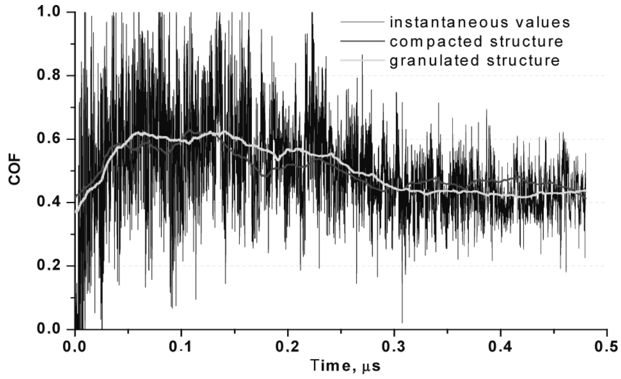

Fig. 3. COF evolution. Black curve indicates momentary COF for the granulated structure and the light grey curve provides the corresponding mean value. The dark grey curve shows mean values for the oxide layer with 13 vol% of graphite inclusions.

4. EXPERIMENTAL RESULTS

The effect of oxide powders on friction and wear of a steel couple has been shown by Kato [11]. A simple pin-on-disc test was described in this paper which clearly showed the effect of different iron oxide powders on COF and wear rate. As an attempt to reproduce such results, we performed almost identical tests with commercially available iron oxide powders. The only difference was that we used cast iron discs as counter bodies and Fe_3O_4 instead of Fe_2O_3. As shown in Fig. 4, this couple provided a mean COF of approximately 0.35, which is considerably lower than the one observed by Kato (0.55). In order to verify the test method we repeated the test with Fe_2O_3 and FeOOH powders. The results were

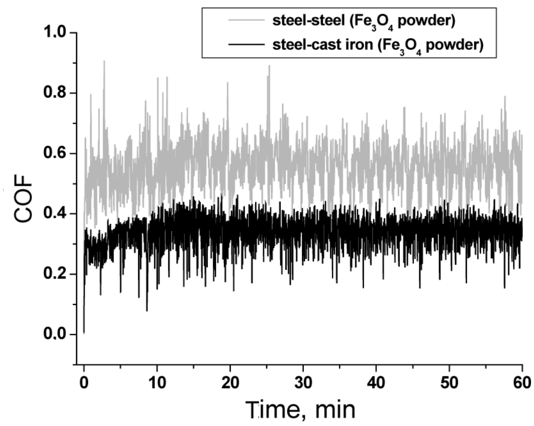

Fig. 4. Results of pin-on-disc tests with Fe_3O_4 supply for cast iron and steel discs. Pin was always steel.

almost identical. Thus we concluded that the difference might be due to the presence of graphite – constituent of the cast iron microstructure – at the interface. Therefore we repeated the tests with counter bodies made of steel St52 in accordance with the description in Kato's paper [11]. Now Kato's result could be reproduced very well, as shown by the upper curve in Fig. 4. The latter result also corresponds well to our modelling results for the oxide layers between steel substrates. On the other hand, the experimental results obtained with the cast iron disc and oxide powder correspond to the behaviour observed by modelling the mixture of oxide with 13 vol% graphite. Thus we conclude that graphite nanoparticles are formed as wear debris of the cast iron which then are mixed with the iron oxide powder.

5. CONCLUSIONS

Despite many simplifications, which were necessary to establish the model, the most important features for braking, namely friction force stabilization and smooth sliding conditions, can be simulated quite well provided that the friction layers have favourable microstructure and composition, which has been identified experimentally.

Thus, in order to provide smooth sliding conditions within dry friction, it is necessary to create conditions that promote the formation of a thin layer of mechanical mixing of the material. According to the simulation, this is achieved by introducing a certain concentration of a soft constituent into the third body layer. It has been proved by modelling as well as by experiments that compact layers and layers of powder particles show similar sliding behaviour and friction levels. Future experiments will focus on quantitative verification of modelling results by preparing artificial third bodies of well defined compositions by high-energy ball milling of iron oxide and graphite powders.

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Kolmanda keha käitumine kuivhõõrdetingimustes. Nanoskaalas modelleerimise võrdlus eksperimendiga

Andrey I. Dmitriev, Werner Österle, Heinz Kloβ ja Guillermo Orts-Gil

Auto piduriklotsid sisaldavad mitmeid koostisosi, kuid seni pole lõplikult selge, milline tähtsus on komposiidis üksikutel elementidel, tagamaks libisemise ererežiime. See on tingitud mehhanismide vastastikusest koosmõjust hõõrdel multiskaalal. Artiklis on tehtud katse leida osaliselt vastus sellele küsimusele, kasutades arvutisimulatsiooni. Kuna simulatsioon lubab arvestada erinevaid süsteemi osade kombinatsioone simuleerimisel, on saanud võimalikuks mõista üksiku koostisosa järjestikust rolli. Põhitähelepanu on pühendatud mõlema keha pinnal tekkivate õhukeste kilede struktuurile ja koostisele ning, silmas pidades kulumisproduktide tihendamist, nende keemilisele koostisele ja oksüdatsioonile.

Hõõrdekile, mida võib ka kolmandaks kehaks nimetada, erineb kahest põhikehast koostiselt ja mikrostruktuurilt. On silmas peetud, et punktkontakt on tasakaaluolekus hõõrdumisel, kui formeerub hõõrdekile struktuur ja koostis. Modelleerimiseks on kasutatud MCA-meetodit (*movable cellular automata*), mis on end seda tüüpi ülesannete lahendamisel õigustanud. Uuriti kolmanda keha struktuuri ja koostise modifitseerimise mõju süsteemi käitumise iseärasustele hõõrdel. Hindamaks arvmudeli adekvaatsust kunstliku kolmanda kehaga, viidi läbi ka vastav eksperiment. Simulatsiooni tulemused olid eksperimentaalsete tulemustega vastavuses.