

Numerical simulation methods in tribology

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Available online 27 March 2006

Abstract

We presented a general structure of a possible reduced description of classical macroscopic tribological systems, which should make it possible to simulate the friction and wear of real systems, taking into account a large variety of relevant processes and space scales, including the contact mechanics and hydrodynamics at macro and meso scales as well as inelastic processes, detachment of particles and their reintegration into the surfaces at the nanoscale. The main features of this reduced description are reduction in the dimensionality of the elastic contact problem from three to one and substitution of the complete hydrodynamics by distance- and velocity-dependent surface forces as well as simulation of inelastic surface processes as stochastic deposition and diffusion along the surface. The processes on the nanoscale are simulated with the method of Movable Cellular Automata.

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Keywords: Tribology; Contact mechanics; Lubrication; Nanoscale; Numerical simulation

1. Introduction

Tribology is a science about bodies in contact in a relative motion. It covers physical processes connected with contact mechanics, friction, lubrication and wear. Applications of tribology range from atomic force microscopy and micromechanical devices over the huge field of macroscopic classical tribology to earthquakes. Tribological systems are so various that any concrete discussion of them is possible only if we define what particular kind of tribological systems we would like to discuss. In this paper, we primarily deal with “traditional” tribological systems, which can be characterized as macroscopic many-contact systems. In spite of the long history of tribology, there are these systems which are poorly understood till now. The striking fact is that the “simple” dry friction between solids cannot be still predicted theoretically in most cases. The reason is in the complexity of processes going on in any tribological contact on different space scales, which can include elastic and plastic deformation of bodies in contact, fracture, detaching of wear particles and their reintegration

into the surfaces, chemical reactions and mechanical alloying.

Another striking property of tribological contacts making them a difficult object is their “multi-scale nature”: in friction processes, both the microscopic and macroscopic scales may play an essential role. Thus, a monolayer of impurity atoms on the metal surface changes dramatically both the friction and wear [1]. On the other hand, the contact mechanics of real surfaces (fractal in most cases) is controlled by space scales differing by many orders of magnitude [2]. The same problems arise in simulation of rubber: the rolling resistance and the wear in this material can be caused by space and time scales differing by about 10 orders of magnitude. A correct simulation has to take into account all these scales [2].

These systems are, however, not completely unpredictable. In fact, the most striking and famous feature of dry friction is that it depends, in the first approximation, neither on the apparent contact area nor on the roughness. As a matter of fact, this is the main reason why we can use the notion of the friction coefficient. This property of dry friction indicates that a relatively simple description of dry friction should be possible, provided that proper theoretical concepts are applied for the analysis.

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The multiscale nature of friction processes makes it necessary to search for possibilities of model reduction, so that any important features of any scale can be properly taken into account. This paper is mainly devoted to the discussion of the possibilities for model reduction and simulation techniques on different scales.

2. Contact aspect of macroscopic tribological systems

Any tribological problem is first of all a contact problem. We begin with a discussion of this contact aspect of tribology. In a typical case, the tribological partners come into contact in a number of microcontacts, with a real contact area much smaller than the apparent area of the contact (Fig. 1). We will show that this gives a possibility to drastically simplify the contact problem.

To describe dynamics of a mechanical system, we need its potential and kinetic energies. We will show that for a typical tribological contact, the space scales contributing to these energies can be clearly separated.

2.1. Potential energy

Let us consider an indentation of a rigid punch with diameter d into an elastic body by the distance $\delta(t)$ with a small velocity $v_0 \ll c$ (c is the sound velocity), so that the deformation process can be considered as a quasi-static one¹ (Fig. 2).

The displacement field in the elastic body far away from the indentation point is in a three-dimensional (3D) system

$$u \simeq \frac{\delta d}{r}. \tag{1}$$

The elastic deformation has the order of magnitude $\varepsilon \simeq (du/dr) \simeq (\delta d/r^2)$. The energy density is of the order of magnitude $E \simeq G\varepsilon^2 \simeq G(\delta^2 d^2/r^4)$. The total potential energy of the elastic deformation is thus

$$U \simeq \int G \frac{\delta^2 d^2}{r^4} 2\pi r^2 dr = 2\pi G \delta^2 d^2 \int \frac{dr}{r^2}. \tag{2}$$

It converges at the upper limit and diverges at the lower limit of integration. As the asymptote (1) is only valid for $r \geq d$, the lower limit should be chosen to be of the order of d . The total potential energy is thus “concentrated” in the volume of the diameter $r \approx d$ and has the order of magnitude

$$U \simeq 2\pi G \delta^2 d. \tag{3}$$

This result can be summarized as follows:

Elastic contact energy is a “local” quantity which only depends on the configuration and deformations in the vicinity of a microcontact, but does not depend on the size and the form of the body as a whole.

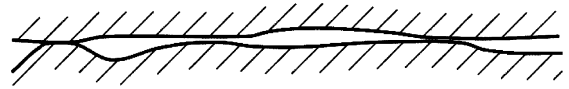


Fig. 1. Contact of two macroscopic bodies.

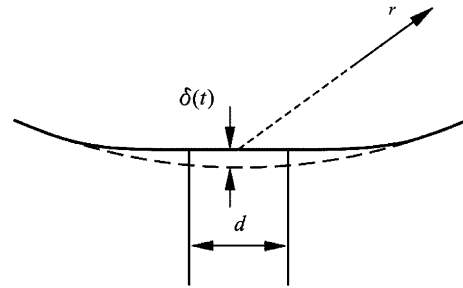


Fig. 2. An indentation of a rigid punch with diameter d into an elastic body by the distance $\delta(t)$.

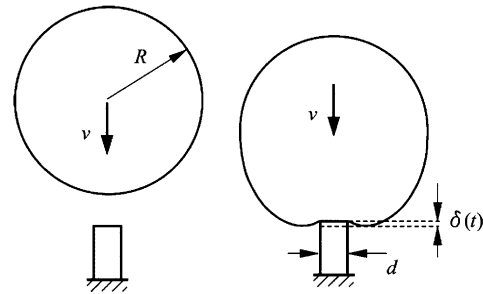


Fig. 3. The body as a whole moving with an average velocity v , coming into contact with an indenter of the diameter d .

2.2. Kinetic energy

Now let us consider the kinetic energy of the medium due to the indentation. The velocity has the order of magnitude

$$v = \dot{u} \simeq \frac{\dot{\delta} d}{r}. \tag{4}$$

If the body as a whole is moving with an average velocity v , and comes into contact with an indenter of the diameter d (Fig. 3), then the kinetic energy of the body will be of the order

$$K \simeq \int \rho \left(v - \frac{vd}{r} \right)^2 \pi r^2 dr \approx \frac{mv^2}{2} \left(1 - \frac{d}{R} \right). \tag{5}$$

If the diameter of the contact is much smaller than the size of the body, the kinetic energy can be in good approximation assumed to be just $mv^2/2$. In this case, the influence of the contact deformations on the kinetic energy can be neglected:

Kinetic contact energy is a “non local” quantity which, in first approximation, does not depend on the configuration of the surface contacts and can be assumed to be equal to

¹This condition is very well fulfilled for most real tribological contacts.

the kinetic energy of a “rigid” motion of the body as a whole.

This conclusion is, however, not valid, if the average velocity of the body is zero (this is, e.g., the case for the vertical component of a sliding velocity for a body sliding in horizontal direction). In this case, the kinetic energy (5) takes the form

$$K \simeq \int \rho \left(\frac{vd}{r} \right)^2 \pi r^2 dr. \tag{6}$$

It converges on the lower limit and diverges on the upper limit. The order of magnitude of kinetic energy is in this case $K \sim mv^2(d/R)^2$, where R is a characteristic size of the body. In this case, the kinetic energy depends both on the shape and size of microcontacts and on the form and size of the body as a whole.

We come to the conclusion that the inertial properties of a “typical tribological system” can be described with respect to the sliding direction just by considering it as a rigid body with a constant mass m (Fig. 4), while with respect to normal direction more complicated consideration is necessary. At the same time, the interactions of a body with other bodies are described completely by the stiffness of microcontacts (or, if not linear, by the exact force–displacement law for each contact). This means a principal possibility of a huge reduction in tribological models.

Note further that the most important factor for the contact interactions between rough surfaces is the distribution of their heights. The elastic interaction between contact areas is of minor importance: thus, the contact theory of Bush [3] neglecting the interaction between asperities, and the theory by Persson [2] neglecting interactions between different scales give practically the same results differing by a constant factor of the order unity. If, however, the elastic interrelation between asperities is neglected, then the dimensionality of the system plays no role any more, provided the necessary statistics of heights are provided and the stiffness of single asperity is the same as in a real 3D system.

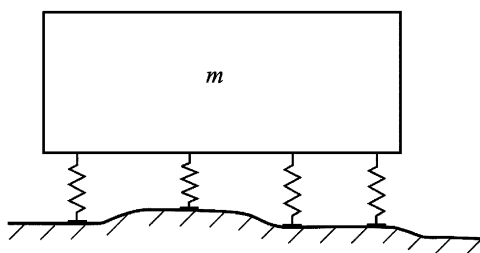


Fig. 4. A typical macroscopic tribological system with respect to the sliding direction can be considered as a rigid body with a constant mass m interacting with its partner by nonlinear spring.

3. Reduction of a 3D contact problem to a 1D problem

The problem of determining the current configuration of microcontacts is a complicated problem because it depends on the whole topography and deformations of both contacting surfaces. The fact that in most cases we are finally interested only in the force–deformation dependence for a single contact leads us to the idea that we do not need to simulate the 3D surface topographies to get the correct contact distribution and stiffness. Indeed, if we manage to become in a 2D or even 1D system, the same contact properties as for the 3D system, it will still properly describe the macroscopic properties of the system, because it is only the force–displacement dependence which is finally of importance for the macroscopic contact problems.

It can be shown that a thin elastic layer on a rigid substrate (Fig. 5b) has in two dimensions the same force–displacement dependence as the 3D contact (Hertz’s problem, Fig. 5a).

This means that a 3D contact problem can be reduced—as far as we are interested in the stiffness of contacts only—to a 1D problem. To prove this, let us consider the nonadhesive contact between two elastic spheres. Hertz theory [4] gives the elastic energy

$$U_{3D} = \frac{4\sqrt{2}G}{15(1-\nu)} \sqrt{Rd^5}, \tag{6}$$

where R is the radius of curvature, d is the penetration, G is the shear modulus and ν is Poisson’s ratio (Fig. 1a). On the other hand, the contact between an elastic layer that is attached to a rigid cylinder (Fig. 1b) and a rigid plane is described by the elastic energy

$$U_{2D} = \frac{2\sqrt{2}c_n}{15} \sqrt{Rd^5}, \tag{7}$$

where c_n is the (constant) stiffness of the springs per unit length. The two expressions are equal if the stiffness is chosen as

$$c_n = \frac{G}{2(1-\nu)}. \tag{8}$$

In a similar way, it is possible to simulate 3D adhesive contacts using 1D systems. This possibility as well as some

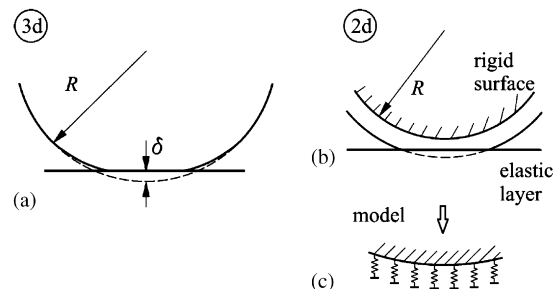


Fig. 5. (a) Force–displacement dependence in the 3D contact (Hertz’s problem). (b) A thin elastic layer on a rigid surface has in two dimensions the same force–displacement dependence as in Hertz’s problem.

restrictions will be discussed in more detail in the paper by Popov et al. in this issue [5].

4. Possibilities of model reduction for elasto-hydrodynamic contacts

Most tribological systems can be characterised as “lubricated” ones. Even in the case of a “dry” friction, there is always some layer of dirt, which plays the role of lubrication. Further, most of solids have at their surface a layer of water of the thickness 10–100 nm, depending on the conditions [6]. We thus normally have to do with a contact of solids with an intermediate liquid layer. Soft layers as leaves in the rail–wheel contact can also be considered approximately as a layer of fluid. Simulation of elasto-hydrodynamic contacts is therefore urgently necessary for understanding friction.

We will show that a similar separation of scales and simplification as in pure elastic contacts can be achieved for elasto-hydrodynamic problems under conditions of mixed lubrication. To illustrate the principal idea, let us consider a motion of a single rigid asperity with radius R towards a rigid plane (Fig. 6).

In Reynolds’ approximation, the gradient of the pressure in the gap between two solids is given by

$$\frac{dp}{dr} = \frac{6\eta r \dot{h}}{h(r)^3}, \tag{9}$$

where $h(r) = h_0 + r^2/2R$ is the thickness of the gap as a function of radius. Integration of (9) gives

$$\begin{aligned} p &= p_0 + \int_{-\infty}^r \frac{6\eta r \dot{h}}{(h_0 + r^2/2R)^3} dr \\ &= p_0 + 6\eta \dot{h} \int_{-\infty}^{(r^2/2R)} \frac{dz}{(h_0 + z)^3} \\ &= p_0 - \frac{3\eta \dot{h}}{(h_0 + r^2/2R)^2}. \end{aligned} \tag{10}$$

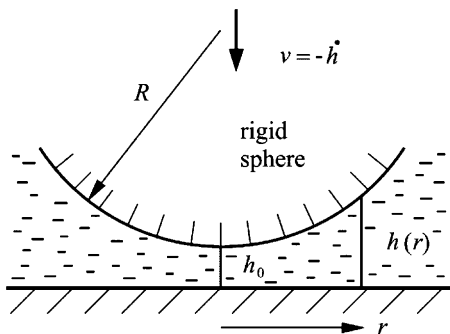


Fig. 6. Motion of a single rigid asperity with radius R towards a rigid plane.

The force acting on the body is equal to

$$\begin{aligned} F &= \int_0^\infty (p - p_0) 2\pi r dr \\ &= - \int_0^\infty \frac{3\pi\eta \dot{h} R^2 dz}{(h_0 + z)^2} = - \frac{3\pi\eta \dot{h} R^2}{h_0}. \end{aligned} \tag{11}$$

The integral giving the force converges on the upper limit. This means that the main contribution to the force gives the immediate vicinity of the microcontact. The details of the flow far away from the contact have no influence on the interaction between asperities.

The force stemming from the tangential motion with velocity v can be estimated as

$$\begin{aligned} F &\sim \eta \int_0^L \frac{v}{h_0 + (r^2/2R)} 2\pi r dr \\ &= 2\pi R \eta v \ln\left(1 + \frac{L^2}{2h_0 R}\right), \end{aligned} \tag{12}$$

with L being the characteristic distance between asperities. This force is much smaller than the normal force (11) and can be neglected in first approximation.

For a rigid contact with curvature radius R the force could be modeled just as a nonlinear damper ($F = -\alpha \dot{h}/h$ with $\alpha = 3\pi\eta R^2$). A generalisation to lubrication with non-Newtonian liquids is straightforward.

Let us show how these ideas can be applied for simulation of lubricated polishing. Consider two surfaces separated by a lubrication layer containing abrasive particles. Provided the particles have some characteristic curvature radius R , the above approach can be developed further. It can be easily shown that the same interaction force (11) can be obtained by introducing a central interaction of surface elements of a particle with surface elements of the one of the solids according to the law

$$dF = \frac{6\eta R}{\pi} \frac{v}{r^4} dA dA', \tag{13}$$

where dA and dA' are surface elements of the sphere and a solid plane, respectively, r is the distance between the elements and v is the projection of their relative velocity onto the direction between them. Integration of force (13) over all elements of the sphere and the plane leads (under the condition $h \ll R$) to Eq. (11). The nonlocal character of the interaction of solids has its manifestation in the explicit dependence of the interaction force on the radius R .

The main advantage of the replacement of the exact interaction over the liquid layer through interaction (13) is that we then do not need to solve the hydrodynamic equations for the lubricant.

In a recent publication, we have shown that this approach can be effectively used for simulating development of surface topography by mechano-chemical polishing of lubricated surfaces [7].

5. Dry friction modeling: what scale is responsible for friction?

The contact problem is of course only the first step of modeling any tribological system. The second step is the friction itself. In this paper, we restrict ourselves to consideration of such tribological systems, where solely elastic interactions among surface heterogeneities *do not* make a significant contribution to the friction force. As is shown in Ref. [1], this is the case if the so-called elastic correlation length of the system is much larger than the body size. This condition is almost always fulfilled for “rigid” bodies (e.g., made of materials with elastic modulus typical of metals) with a length of the tribological contact about a few centimeters. The absence of elastic contribution to the friction force implies that in the case where the bodies are absolutely elastic and absolutely smooth (in the sense of zero friction at the micro level), the macroscopic friction force would be zero. This is due to the fact that elastic forces acting from micro-heterogeneities of one body on the micro-heterogeneities of the other are randomly directed; if no elastic instabilities occur in contacts (this is the case for any body whose size is smaller than the elastic correlation length), their averaging takes place and the macroscopic friction force is zero. The physical cause of friction forces for the foregoing contacts must, therefore, lie at a lower-scale level and be due to the processes of inelastic deformation of surface volumes. It is important to determine this scale. This is not a purely theoretical problem but an experimental one.

To determine the scale responsible for the friction force in different materials, we have developed a special measuring method called tribospectroscopy. The idea of the method is the following. We consider a sample with a length which can oscillate with high frequency due to built-in piezo elements [8,9] (Fig. 7). Theoretical prediction is [10] that the friction law should undergo essential changes, if we let oscillate the sample with an amplitude comparable with the intrinsic scale of friction processes. By oscillating, we “probe” in some sense the scale comparable with the oscillation amplitude. By measuring the friction force of a body oscillating with different amplitudes, we can receive information about all the scales probed in such a way.

In the experiments described below [8], a steel probe has been used, contacting a supporting plate in two small contact areas at its ends (Fig. 7). The length of the probe could be changed due to piezo elements built in at the

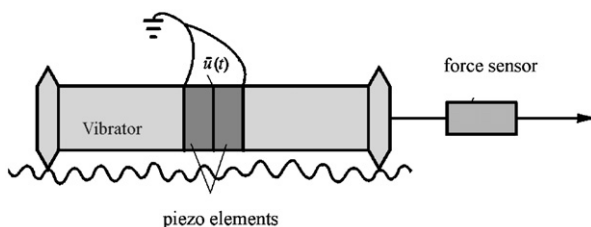


Fig. 7. Scheme of the experimental setup.

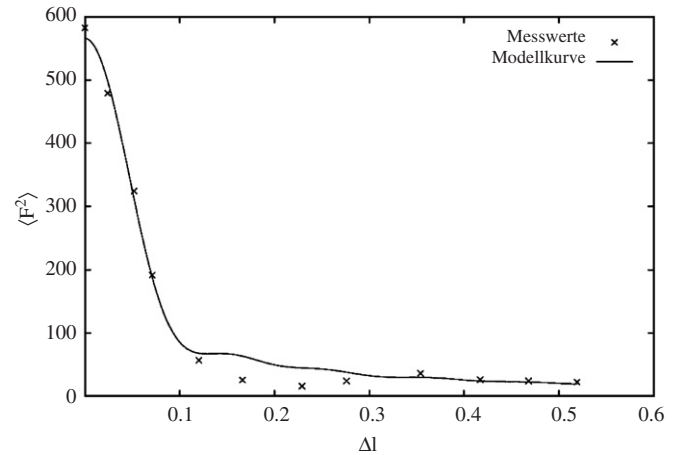


Fig. 8. Dependence of the square of the friction force on the oscillation amplitude of the probe. The solid line is a theoretical curve according to Eq. Experimental results: \times , theoretical curve: —. From Ref. [8].

middle of the probe. The piezo elements have been driven by an alternate voltage at a frequency around 60–70 kHz. The oscillation amplitude $\Delta l/2$ of one side surface of the probe was measured via a laser Doppler measuring device.

The experimental results are shown in Fig. 8. The friction force decreases rapidly in the interval of oscillation amplitudes from 0 to 0.1 μm and then shows only a moderate decrease up to the amplitudes of about 0.5 μm . Comparison with theory shows that the characteristic space scale giving rise to the friction force in this tribological system is of the order of magnitude of 50 nm. (Fig. 8)

The absence of a pure elastic contribution to the friction force as well as the experimentally determined relevant space scale of friction processes shows that we have to investigate inelastic processes on the space scale of about 50–100 nm.

6. Modeling friction on the nano scale: method of movable cellular automata (MCA)

The processes occurring in tribological contacts on the scale of about 100 nm are elastic and plastic deformations, fracture, detachment of nanoparticles and their reintegration in one of the contacting surfaces as well as intensive mechanical alloying. Application of numerical methods based on discretization of continuum models (FEM, BEM) is in this case either difficult or rather impossible.

To model the processes in the surface layers, we use the method of MCA [11–13]. According to this method, a medium is represented as an ensemble of discrete elements—MCA characterized by continuous variables such as center of mass position, value of plastic deformation, rotation pseudo-vector as well as by the discrete variables characterizing connectivity of the neighboring automata. The principles of writing the equation of motion for a system of cellular automata and prescribing interactions between them are described in Ref. [12].

We present one example of simulation of friction processes with the MCA method. We investigated an object consisting of four parts (Fig. 9):

- The upper layer of automata was an absolutely rigid, nondeformable body moving horizontally at velocities v ranging between 1 and 20 m/s in different numerical experiments.
- Two intermediate layers with initial roughness of nanometer range represented surface regions of the bodies in contact.
- The lower layer was a fixed support.

A constant normal force corresponding to the pressure range between $P = 0.5$ and 382 MPa acted upon all the elements of the upper layer. The diameter of the automata was from 2.5 to 10 nm in different numerical experiments. The elastic properties of the automata corresponded to the steel with Young's modulus of $E = 206$ GPa and Poisson's ratio $\nu = 0.3$. The yield strength σ_{y1} and ultimate strength with respect to tension σ_0 were varied between 80 and 480 MPa and between 92 and 552 MPa, respectively.

An important parameter determining stability of the plastic deformation processes and significantly affecting the characteristic size of the surface region of the severe plastic deformation is viscosity. Phenomenological viscosity reflects dissipation processes under strain occurring due to electron and phonon excitation in a solid. It was assumed in the numerical model that viscous forces acting between unconnected but contacting automata are proportional to the relative velocity of motion. At the left and right fragment boundaries, periodic boundary conditions were used. The initial roughness was specified in the explicit form.

6.1. Formation of a boundary “quasi-liquid” layer

The numerical experiments show that already within first nanoseconds after onset of a relative tangential motion of bodies, the roughness of both surfaces is severely deformed and fractured, and a dynamic equilibrium in the system is established at a temporal scale of about 100 ns. A pronounced boundary layer appears, where the processes of deformation, fracture, reconstruction of connectivity between elements and intensive mixing take place. The motion in the layer resembles turbulent motion in liquid (Fig. 9b). For this reason we refer to it as a “quasi-liquid layer”. Note, however, that this layer is not liquid in terms of thermodynamics. A quasi-liquid layer remains localized in the vicinity of the initial friction surface and does not propagate to deeper regions of the contacting bodies.

A characteristic depth of the layer depends on the system parameters; first and foremost, on the effective viscosity of the system of automata. In our calculations, viscosity was used as a fitting parameter and was chosen so that the layer depth corresponded to the experimental values [16]. Any particular form of the initial roughness does not influence the results of simulation.

The method of MCA allows one to simulate the friction force as a function of material and loading parameters [14], development of surface topography [17] and wear [13,15].

7. Simulation of development of surface topography

As already mentioned, the contact between bodies usually occurs at a small number of microcontacts. If the bodies are in a relative tangential motion, the positions of microcontacts rapidly (and stochastically) change. It is important to note that even if the probability to have a

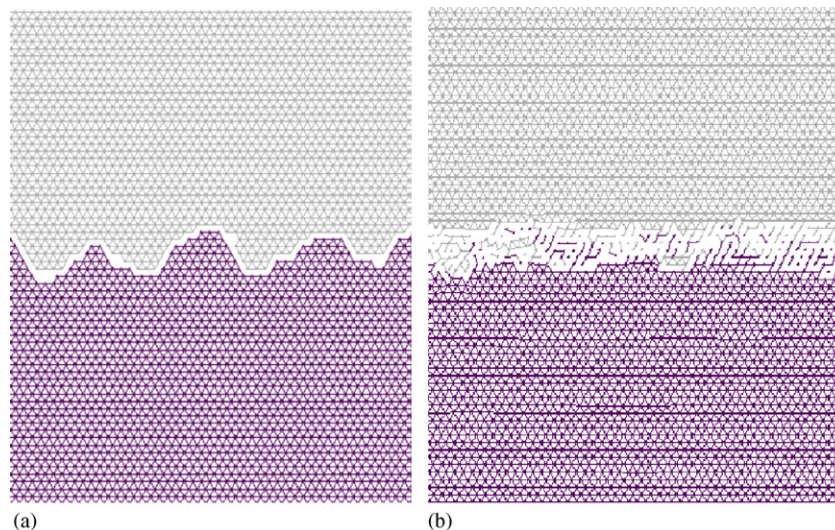


Fig. 9. Formation of a quasi fluid layer in friction: simulation with MCA.

contact at a “hill” is larger than in a “valley” of the surface, there is a finite probability of contacts along the whole surface (because the “hills” of one surface can contact the “valley” regions of the other). The irreversible processes of plastic deformation and fracture due to “impacts” between surfaces therefore occur in a stochastic manner in the rapidly changing points of the surface. The processes in microcontacts giving rise to irreversible changes of the surface topography are plastic deformation, detaching of wear particles and their reintegration into the surfaces. Plastic deformation leads to a mass transport *along* each surface, while the detaching and reintegration processes lead to a mass transfer *between* the contacting surfaces. Both processes can be macroscopically modeled as a stochastic transport of material either *along* the surface or *to* and *from* the surface. This picture of a stochastic mass transport can be used as a basis for a simple phenomenological model of processes leading to changes in surface topography.

The stochastic transport along the surface due to plastic deformation or repeated detaching and reintegration of wear particles into the same surface can be described as a stochastic wandering of “particles” (surface elements of the body) with some distribution of mass, length and time of the elementary transport process. It is known that such stochastic transport of many elements can be macroscopically described by a diffusion equation. Note that here we mean an effective diffusion of mass due to stochastic wandering and *not* molecular diffusion at the atomic scale. The diffusion coefficient is known to be equal to $D \simeq (l^2/\tau)$, where l is the characteristic length of an elementary step and τ is its characteristic time. To formulate a mathematical model of stochastic mass transport, we should be able to make statements about the characteristic length and times of elementary acts of stochastic transport.

The second process is the mass transfer from one rubbing body to the other. This process can also be described as stochastic detaching and deposition from and onto the surface.

It is important to note that a macroscopic description of stochastic transport as a diffusion process is only possible if a characteristic microscopic space and time scale of elementary processes exists. Thus the diffusion approach is only valid on space scales much larger than this microscopic scale. The existence of such microscopic scale for the mass transport in friction follows from the concept of a *quasi-fluid layer* at the surface of rubbing bodies as described in the previous section. The existence of this layer substantiates the “diffusion model” of mass transport by introducing the required microscopic length parameter.

Let us denote the height of the surface measured from the average level by h . We can think of the material as an assembly of elements with characteristic sizes of about l piled over each other. The height h is proportional to the amount of material at the given coordinate x of the surface. The diffusion equation describing the stochastic mass

transport has the form

$$\dot{h}(x, t) + \frac{\partial}{\partial x} j(x, t) = 0, \quad (14)$$

where the dot denotes the usual time derivative and

$$j(x, t) = -D \frac{\partial}{\partial x} h(x, t) \quad (15)$$

is the flux density of particles. With (15), Eq. (14) can be rewritten as

$$\dot{h}(x, t) = D \frac{\partial^2}{\partial x^2} h(x, t). \quad (16)$$

If the distribution of heights was initially heterogeneous, it will be “flattened” in the course of time due to the effective diffusion processes of particles from the hills to the valleys. However, Eq. (16) describes the average result of diffusion only. On the micro scale, the micro impacts lead to a *roughening* of the surface. This microscopic random noise can be modeled if we modify the flux term (15) by introducing the noise caused by individual impacts. This can be done by adding a stochastic flux

$$j_s = l f_x(x, t), \quad (17)$$

where $f_x(x, t)$ is a stationary Gaussian-distributed noise in space and time and l is a characteristic length scale introduced for dimensional reasons. Since Eq. (14) has the form of a continuity equation, a stochastic flux does not change the total mass of the surface, it merely describes the effect of microscopic plastic deformation, i.e., rearrangements of particles of the same surface. The noise is assumed to have the following autocorrelation functions:

$$\begin{aligned} \langle f_x(x, t) \rangle &= 0 \\ \langle f_x(x, t) f_x(x', t') \rangle &= 2D_x F(x - x') \delta(t - t'). \end{aligned} \quad (18)$$

The spatial correlation function $F(x - x')$ includes a correlation length l_c that defines the microscopic scale on which the stochastic impacts occur. We will always assume that $l_c \ll l$. The diffusion coefficient D_x defines the “strength” of the noise, which is a measure for the intensity of the plastic deformation process.

The transfer of particles *between* surfaces includes two main processes.

Firstly, we model the abrasive wear that is induced by repeated contacts of surface asperities. Elementary wear events occur with a certain probability. The higher the asperities, the more likely a wear event is. The change of height in time is

$$\dot{h}(x, t) = -\mu h(x, t), \quad (19)$$

where the phenomenological constant μ is introduced.

Secondly, we note that this process is superimposed by stochastic impacts of wear particles that are detached or reintegrated into the surface on the micro scale, thus processes connected with adhesion. This is modeled by a second stochastic, Gaussian-distributed force $f_z(x, t)$ with

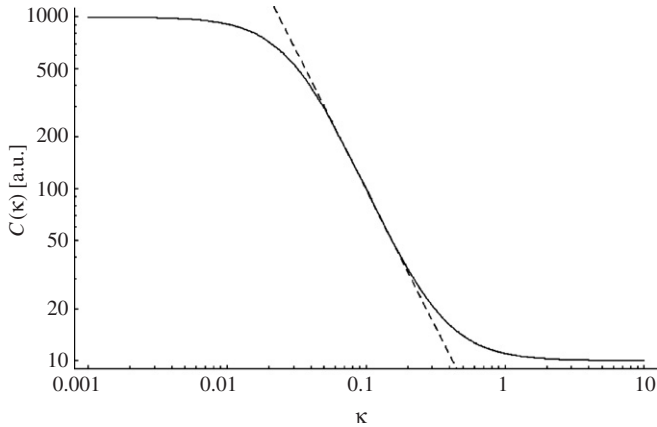


Fig. 10. Power spectrum. The dotted line shows the fractal κ^{-2} behavior. From Ref. [18].

the correlation functions

$$\begin{aligned} \langle f_z(x, t) \rangle &= 0 \\ \langle f_z(x, t) f_z(x', t') \rangle &= 2D_z F(x - x') \delta(t - t'). \end{aligned} \quad (20)$$

Since the particles responsible for the plastic deformation described above are the same that can be integrated into the surface or detached from it, this noise has the same spatial correlation $F(x - x')$, but a different diffusion constant $D_z \neq D$. The stochastic change of height in time

$$\dot{h}(x, t) = f_z(x, t) \quad (21)$$

describes the vertical transfer of particles between the surfaces, with a mean intensity defined by

$$D_z = \frac{l^2}{\tau_z}, \quad (22)$$

where a new time scale τ_z has been introduced.

Putting all pieces of the model together, the diffusion Eq. (16) is generalized by adding the stochastic flux (17) describing plastic deformation, the wear process (19) due to contacts of asperities and the stochastic detachment and reintegration of wear particles (21), yielding

$$\begin{aligned} \dot{h}(x, t) = \frac{\partial}{\partial x} \left(D_0 \frac{\partial}{\partial x} h(x, t) + l f_x(x, t) \right) \\ + f_z(x, t) - \mu h(x, t). \end{aligned} \quad (23)$$

A typical equilibrium power spectrum resulting from this equation is shown in Fig. 10. This power spectrum has two plateaus. The slope of the spectrum between these plateaus shows the fractal κ^{-2} behavior that is inherent in most surfaces.

8. Conclusions

We presented a general structure of a possible reduced description of classical macroscopic tribological systems, which should make it possible to simulate the friction and wear of real systems, taking into account a large variety of

relevant processes and space scales, including the contact mechanics and hydrodynamics at macro and meso scales as well as inelastic processes, detachment of particles and their reintegration into the surfaces at the nanoscale. The main features of this reduced description are reduction in the dimensionality of the elastic contact problem from three to one and substitution of the complete hydrodynamics by distance- and velocity-depending surface forces as well as simulation of inelastic surface processes as stochastic deposition and diffusion along the surface. The force and diffusion laws should be modeled at the nanoscale by the method of MCA. Some further steps towards a general simulation technique for friction processes are presented in other papers of this special issue.

References

- [1] BNJ Persson. Sliding friction. Physical principles and applications, second ed. New York: Springer; 2000. 516p.
- [2] Persson BNJ, Albohr O, Tartaglino U, Volokitin AI, Tosatti E. On the nature of surface roughness with application to contact mechanics, sealing, rubber friction and adhesion. *J Phys: Condens Matter* 2005;17:R1–R62.
- [3] Bush AW, Gibson RD, Thomas TR. *Wear* 1975;35:87.
- [4] Landau LD, Lifschitz EM. Theory of elasticity, third ed. London: Pergamon Press; 1986.
- [5] Popov VL, Geike T, Filippov AE. A model of friction of flexible surfaces (this issue).
- [6] Scherge M, Gorb S. Biological micro- and nanotribology. Nature's solutions. Berlin: Springer.
- [7] Popov VL, Filippov AE. Modeling of processes of mechanical polishing with lubrication. *Tech Phys Lett* 2005.
- [8] Popov VL, Starcevic Ya. Tribospectroscopic study of a steel–steel friction couple. *Tech Phys Lett* 2005;31(4):309–11.
- [9] Popov VL, Dudko OK. Tribospectroscopy of surfaces with random roughness. *JTP Lett* 2004;30(4):42–8.
- [10] Dudko OK, Popov VL, Putzar G. Tribospektroskopie fraktaler Oberflächen. *Tribologie Schmierungstech* 2004;5:23–6.
- [11] Psakhie SG, Horie Y, Ostermeyer GP, Korostelev SYu, Smolin AYU, Shilko EV, et al. Movable cellular automata method for simulating materials with mesostructure. *Theoret Appl Frac Mech* 2001;37(1–3): 311–34.
- [12] Popov VL, Psakhie SG. Theoretical foundations of simulation of elastoplastic media with the method of movable cellular automata. I. Homogeneous media. *Phys Mesomech* 2001;4(1):15–25.
- [13] Popov VL, Psakhie SG, Gerve A, et al. Wear in combustion engines: experiment and simulation by the method of movable cellular automata. *Phys Mesomech* 2001;4(4):73–83.
- [14] Popov VL, Psakhie SG, Shilko EV, Knothe K, Bucher F, Ertz M. Friction coefficient in “rail-wheel”-contacts as a function of material and loading parameters. *Phys Mesomech* 2002;5(3):17–24.
- [15] Popov VL, Psakhie SG, Dmitriev A, Shilko E. Quasi-fluid nanolayers at the interface between rubbing bodies: simulation by movable cellular automata. *Wear* 2003;254(9):901–6.
- [16] Popov VL, Smolin IYu, Gervé A, Kehrwald B. Simulation of wear in combustion engines. *Comput Mater Sci* 2000;19(1–4):285–91.
- [17] Dmitriev AI, Popov VL, Psakhie SG. Simulation of surface topography with the method of movable cellular automata. *Tribol Int* 2005;39(5):444–9.
- [18] Schargott M, Popov V. Diffusion as a model of formation and development of surface topography. *Tribol Int* 2006;39(5):431–6.