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A Model of Mechanical Polishing in the Presence of a Lubricant

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Abstract—Modeling of the friction and wear at the contact of rough surfaces in the presence of a lubricant is important for the development of modern technologies. This is a complex problem involving a consistent description of the elastic straining of contacting bodies and of the flow of viscous liquid between them. It is demonstrated that this problem can be significantly simplified in the most interesting case, in which the lubricant thickness is very small and the decisive contribution to both the contact interaction and the friction force is due to the interactions between a finite number of inhomogeneities approaching one another to a certain distance, this distance being much smaller than the average distance between the two bodies. The lubricant dynamics can be modeled in terms of the nonconservative interactions between the particles, which depend on the distance and relative velocity. The proposed approach is used to describe the process of mechanical polishing in the presence of abrasive particles suspended in the lubricant layer. This hydrodynamic polishing process results in the formation of a surface relief with a statistically equilibrium roughness that exhibits a fractal character.

In recent years, the task of obtaining high-quality surfaces with the desired parameters of both a macroscopic inhomogeneity and a microscopic roughness has become very important. The problem of creating such surfaces is encountered, for example, in the production of magnetic disks and integrated chips. The solid surfaces are frequently processed using the method of chemical-mechanical polishing [1], according to which the disk of a polished material (e.g., silicon wafer) is brought into contact with a rotating substrate via a lubricant layer. The lubricant layer may contain suspended abrasive particles. In the typical regime, the abrasive particles do not have direct contacts with the surface of a processed material. Irreversible changes in the surface topography are caused by fluctuations of the pressure developed in a thin lubricant layer separating the abrasive particles and the processed surface. The laws of such a "hydrodynamic polishing" process have not been theoretically studied until now.

This Letter describes a model of the process of surface topography variation as a result of the interaction with abrasive particles suspended in the lubricant layer. In order to increase the efficiency of the numerical model, we have developed a new approach to the description of the hydrodynamic interaction. According to this, the interaction mediated by a liquid layer can be modeled without solving the corresponding hydrodynamic problem. The proposed approach is used to model the process of friction at the contact of two rough surfaces in the presence of a lubricant layer.

Hydrodynamic forces at a single contact. In the aforementioned problem of hydrodynamic polishing, we deal with a system in which the average distance between the two surfaces is much greater than the minimum distance to which the abrasive particles approach the processed surface at a "contact" site. As will be shown below, the main contribution to the interaction force in this case is related to the small vicinity of the point of maximum approach. Taking this into account, we can reduce the description of the interaction between two surfaces to the description of forces arising in pairs of such microcontacts in the presence of a liquid. A single microcontact will be modeled using a hard spherical surface of radius R, which approaches a plane. Since the main contribution to the force is related to the small vicinity of the point of maximum approach, the hydrodynamics in the liquid layer can be considered using the Reynolds approximation [2].

The idea of the proposed approach can be illustrated using the following example. Consider a hard sphere of radius R approaching at a small velocity a solid plane in a liquid medium (Fig. 1). The distribution of pressure in the liquid medium in the Reynolds approximation is described by the equation

$$\frac{dp}{dr} = -\frac{6\eta r\dot{h}}{h(r)^3}, \tag{1}$$

where η is the dynamic viscosity of the liquid, r is the polar radius measured from the point of maximum approach, and $h(r) = h_0 + r^2/2R$ is the distance from a point on the spherical surface to the plane. Integrating

Eq. (1), we obtain an expression describing the pressure distribution in the liquid:

$$p = -\int \frac{6\eta r\dot{h}}{h(r)^3}dr = -\int \frac{6\eta r\dot{h}}{(h_0 + r^2/2R)^3}dr$$
$$= \frac{3\eta \dot{h} R}{(h_0 + r^2/2R)^2} + p_\infty. \quad (2)$$

The total force with which the liquid acts upon the sphere is

$$F = \int (p(r) - p_\infty)dr = \int_0^{-R} \frac{4\eta \dot{h} R}{(h_0 + r^2/2R)^2} 2\pi r dr.$$

Since the integral in (2) converges at the upper limit, this limit can be replaced by the infinity:

$$F \approx \int_0^{\infty} \frac{3\eta \dot{h}}{(h_0 + r^2/2R)^2} 2\pi r dr = \frac{6\pi\eta \dot{h} R^2}{h_0}. \quad (3)$$

The convergence of this integral implies that regions occurring sufficiently far from the contact (at distances much greater than $r \approx \sqrt{2Rh_0}$) practically do not contribute to the interaction between the two surfaces. Therefore, it is necessary to determine only the character of flow in the immediate vicinity of the point of maximum approach.

Using Eq. (3), we can determine the force of interaction between two rough surfaces via the liquid layer without solving hydrodynamic equations—merely by determining the statistics of the heights and curvature radii of the microscopic roughnesses and summing the forces given by formula (3) over all the pairs of closely spaced roughnesses (or roughnesses and suspended abrasive particles).

The proposed approach can be further developed in application to the case where the interacting particles can be characterized by a certain radius of curvature. Equation (3) shows that the force of interaction between a sphere and a solid plane is proportional to the relative velocity and inversely proportional to the distance between the two surfaces. It can be readily shown that the same relation is observed in the case of a central interaction between elements of the spherical surface and elements of the plane according to the law

$$dF = \frac{6\eta R}{\pi} \frac{v}{r^4} dA dA', \quad (4)$$

where dA and dA' are the surface elements of the sphere and the plane, respectively; r is the distance between these elements; and v is the velocity of their mutual approach. The integration of force (4) over all the elements of the sphere and the plane under the condition $h \ll R$ leads to relation (3). The nonlocal character of the interaction of solids via the liquid layer is manifested by the explicit dependence of the interaction force on the radius R.

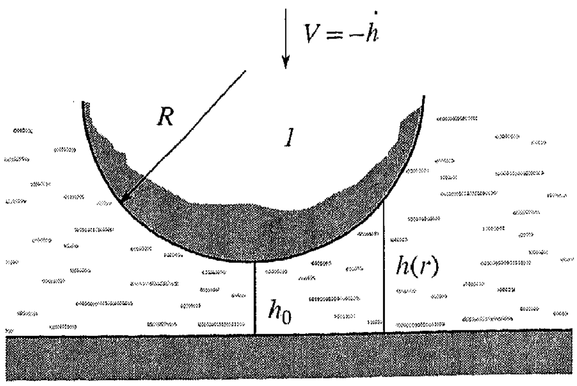

Fig. 1. A model of the microscopic contact between a hard spherical particle (*1*) and a solid surface.

The main advantage of passing from the exact interaction via liquid to the central interactions (4) consists in the possibility of modeling friction between randomly rough surfaces without solving the hydrodynamic equations.

Description of model. Below we consider the simplified discrete model of elastic bodies schematically depicted in Fig. 2. The model represents a series of equidistant material points elastically bound to a hard surface possessing a preset profile. It will be assumed that the surfaces interact only via particles suspended in the lubricant layer. As was demonstrated above, this interaction can be described using forces of the type given by formula (4), which depend on the distances between particles and on their relative velocities. Inelastic interactions between the particles and surfaces will be described as follows: if the force acting upon a particle on the surface exceeds a preset yield point, the "seeding" profile exhibits a depression or protrusion, depending on the sign of this pressure.

A system of dynamic equations for the model described above can be written as follows:

$$\partial v_{z1,2}/\partial t = K_z(w_{1,2}(x) - z_{1,2}(x)) + K_z(z_{1,2}(x+dx)$$
$$+ z_{1,2}(x-dx) - 2z_{1,2}(x)) - F^{(1,2)}_{z\,\text{liquid}} - F^{(1,2)}_{z\,\text{repuls}}. \quad (5)$$

$$\partial V_{x,z}/\partial t = \sum_{(1,2)} [F^{(1,2)}_{x,z\,\text{liquid}} + F^{(1,2)}_{x,z\,\text{repuls}}] - F_{x,z\,\text{diss}}$$
$$+ D\zeta(X, Z),$$

where $\partial X/\partial t = V_x$; $\partial Z/\partial t = V_z$; $\partial x_{1,2}/\partial t = v_{x1,2}$; $\partial z_{1,2}/\partial t = v_{z1,2}$; K_z is the elastic constant of bonds between

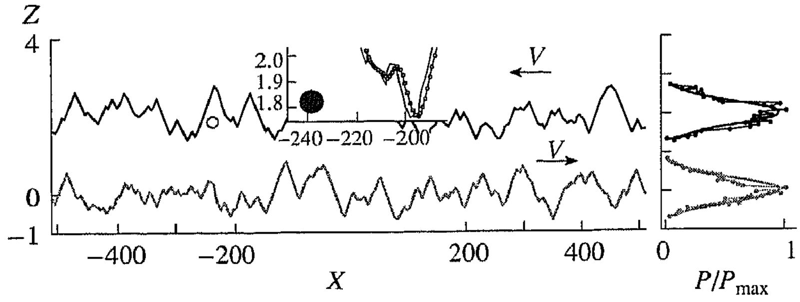

Fig. 2. A discrete model of the contact between two elastic rough surfaces. The diagram shows a fragment of the two-dimensional (x, z) section with the hard "seeding" profiles of the upper (black curve) and lower (gray curve) surfaces. Arrows indicate the directions of motion. The central inset shows deviations of the material points (small black circles) from the seeding profiles. The big black circle shows an abrasive particle suspended in the lubricant layer, which produced these deviations. The right-hand inset shows the instantaneous (points) and time-averaged (solid curves) distributions of the heights of both surfaces obtained as a result of polishing.

mobile elements (material points) of the upper and lower surfaces in positions with the coordinates $z_{2,1}(x)$, respectively, and the quasi-static "seeding" profiles $w_{2,1}(x)$ of the same surfaces; and the sum $\Sigma_{(2,1)}$ is taken over all elements of both surfaces. In addition, we take into account the intrinsic elasticity of these surfaces, which will be roughly approximated by the elastic bonds $K_z(z_{1,2}(x+dx) - z_{1,2}(x))$ (with the same elastic constant K_z as above) in the sequence of surface elements spaced by dx on each surface.

If the absolute value of the difference $|w_{1,2}(x) - z_{1,2}(x)|$ exceeds the yield point W, the surfaces $w_{2,1}(x)$ exhibit a relatively small plastic deformation. According to the proposed model, this deformation is described using the relations

$$w_{2,1}(x) = w_{2,1}(x) \quad \text{for} \quad |w_{2,1}(x) - z_{2,1}(x)| < W;$$
$$w_{2,1}(x) = \mu w_{2,1}(x) + v z_{2,1}(x) \qquad (6)$$
$$\text{for } |w_{2,1}(x) - z_{2,1}(x)| > W,$$

where $\mu + v = 1$ and $\mu/v \gg 1$. These relations should be considered jointly with Eqs. (5).

With neglect of the interactions between particles occurring between the surfaces, we may consider the result of the joint action of particles upon these surfaces as produced by a single particle in a certain statistical realization of the process (with averaging over a long time of the numerical experiment or over multiply repeated realizations). The coordinates of this particle will be denoted (X, Y).

The interaction of a particle with elements of the surface is a sum of the aforementioned liquid friction $F^{(1,2)}_{x,z\,\text{liquid}}$ and the repulsion between this point and the surface elements. For simplicity, the repulsion potential can be set as a Gaussian function of the distance, $U_{1,2} = C c\exp\{-[(X - x_{1,2})^2 + (Z - z_{1,2})_2]/c\}/2$, such that $F^{(1,2)}_{x\,\text{repuls}} = -\partial U_{1,2}/\partial x$ and $F^{(1,2)}_{z\,\text{repuls}} = -\partial U_{1,2}/\partial z$.

The temperature fluctuations must also be taken into account (as usual, within the framework of the Langevin equation) by introducing a δ-correlated random force $D = 2k_BT\eta$ $(\langle\zeta(X, Z; t)\zeta(X', Z'; t)\rangle = D\delta(X' - X')\delta(Z' - Z')\delta(t' - t'))$ and a dissipation with the intensity proportional to the difference between velocities of the particle and each surface $F_{z\,\text{diss}} = \eta V_z$; $F^{(1,2)}_{z\,\text{diss}} = \eta(V_x \pm V)$.

For the symmetry (which increases the accuracy of numerical experiments in the case under consideration), we assume that the upper and lower surfaces move with equal velocities V in the opposite directions as shown in Fig. 2. In this case, the lateral dissipative force is $F_{x\,\text{diss}} = \eta(V_x + V) + (V_x - V) = 2\eta(V_x)$.

We will use the mirror boundary condition for the particle in the Z direction. According to this condition, the particle going outside the interval between $\langle w_2(x)\rangle$ and $\langle w_1(x)\rangle$ is returned back with the same value and opposite direction of the velocity V_z. The boundary conditions in the X direction are periodic.

The formation of equilibrium friction surface. The results of numerical experiments using the model described above showed that the local collisions of abrasive particles with the surface inhomogeneities lead to a continuous change in the surface topography with the formation of a certain equilibrium roughness. If a numerical experiment starts with smooth surfaces, they eventually become rough. Figure 3 shows the typical example of a quasi-random walk of an abrasive particle suspended in a lubricant layer (occurring at the origin at $t = 0$). This motion resembles at first glance the usual diffusion, but a more thorough analysis shows that the diffusion should be considered as anomalous. The main sign of the anomalous diffusion is the presence of long jumps (ballistic flights) [3–5].

In the case under consideration, these ballistic flights have both a simple meaning and large practical significance. Indeed, statistical analysis shows that the flights are related to periods in which the particle approaches significantly closer to the upper or lower

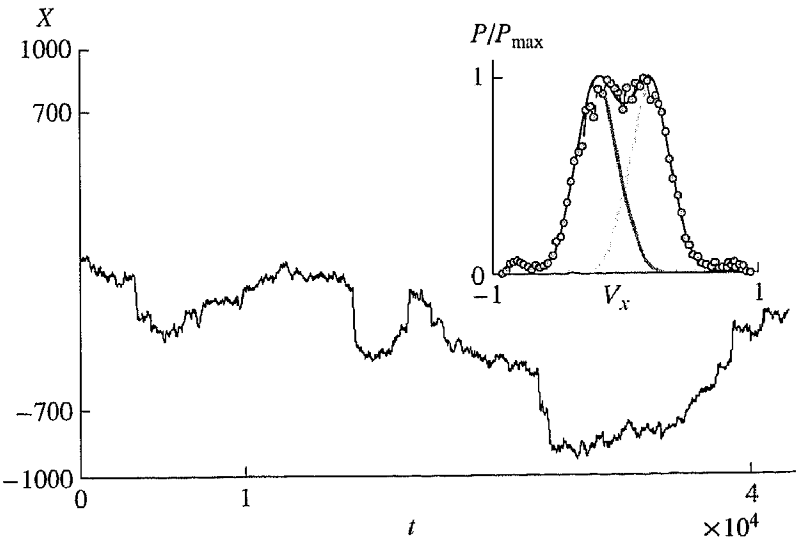

Fig. 3. The typical scenario (time series) of a quasi-random walk of an abrasive particle suspended in a lubricant layer (occurring at the origin at $t = 0$). The inset shows the distribution of the instantaneous particle velocities $P(V_x)$ (open circles) accumulated for the given time series, the distribution averaged over the ensemble (thick solid curve), and the distributions corresponding to the periods of motion when the particle moves predominantly together with the upper (thin solid curve) or lower (gray curve) surface.

surface and, accordingly, more intensively interacts with the surface. In these states, the particle moves together with the corresponding surface and may stray a rather large distance from the initial position. This circumstance is substantially related to the liquid friction in the system with lubricant, which significantly increases the intensity of liquid stirring and, hence, the efficiency of the polishing process.

These considerations are illustrated in the inset to Fig. 3, which shows the distribution of the instantaneous particle velocities $P(V_x)$ (open circles) accumulated for the particular time series of diffusion presented in Fig. 3. For the comparison, we also present the distribution $P(V_x)$ averaged over the ensemble (thick solid curve) and the distributions corresponding to the periods of motion when the particle moves predominantly together with the upper (thin solid curve) or lower (gray curve) surface.

The irreversible changes of surface topography described by relations (6) lead to a constant shift of the surfaces in the opposite directions along the Z axis, which reflects the wear that has occurred as a result of polishing (or a total shift $dZ < 0$ necessary to maintain the constant spacing between the surfaces). Accumulating the shift, we obtain the dependence $dZ(t)$ reflecting the wear that has occurred at a practically constant rate in the course of polishing (Fig. 4). The inset to Fig. 4 shows the distribution of the probability of finding the particle at a point with the coordinate Z between the plates (the data were accumulated for the same particular scenario as that used to determine the $dZ(t)$ dependence). As can be seen, the particle occurs predominantly in the immediate vicinity of each surface and rather frequently enters the regions where it is on the average close to one or another surface. This behavior increases the intensity of polishing and is consistent with the aforementioned mechanism of anomalous diffusion.

One of the most important characteristics of the process under consideration is the spectral structure $C(q)$ of the quasi-equilibrium surfaces formed as a result of polishing. The results of multiply repeated numerical experiments performed in a broad range of the parame-

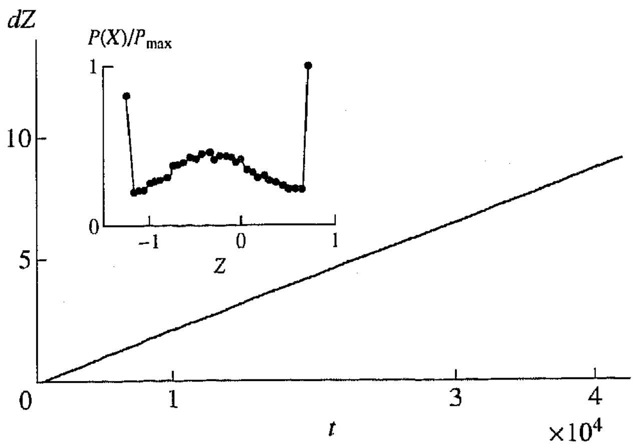

Fig. 4. The wear of surfaces caused by their interaction with an abrasive particle suspended in the lubricant layer (for the time series presented in Fig. 3). The function $dZ(t)$ reflects the total accumulated shift of the average positions $z_{1,2}$ over the time t, which is necessary to maintain a constant average spacing between the polished surfaces. The inset shows the distribution of the probability of finding the particle at a point with the coordinate Z between the plates for the same time series.

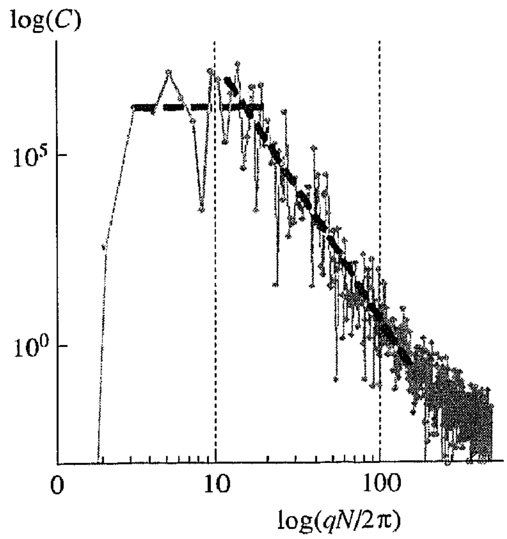

Fig. 5. The typical spectral density curve $C(q)$ for quasi-equilibrium surfaces obtained as a result of polishing. Such a density spectrum is typical of a broad class of real surfaces [6]. In the region of the variable q between the vertical dashed lines, the $C(q)$ function exhibits a scaling behavior, with the range of scales from 10 to 100 units of length dx in the real space.

ters of Eqs. (5)–(6) showed that such surfaces are stably formed within the framework of this model under rather arbitrary initial conditions (flat plates, surfaces generated by random throwing, or surfaces determined by certain spectral structures).

Figure 5 shows the typical spectral density curve $C(q)$ for quasi-equilibrium surfaces $z_{1,2}$ obtained as a result of polishing. Such a density spectrum is typical of a broad class of real surfaces [6]. In particular, the given profile contains a well-pronounced region of the variable q where the $C(q)$ function exhibits a scaling behavior. This region (indicated by vertical dashed lines in Fig. 5) corresponds to the scales from 10 to 100 units of length dx in the real space.

Conclusion. We have developed a new effective approach to the modeling of the elastic-hydrodynamic contacts between rough solid surfaces and of the process of surface topography variation during friction. It was demonstrated that the relative motion of two bodies separated by a lubricant layer containing suspended abrasive particles leads to the formation of statistically equilibrium surfaces with a characteristic fractal topography. The proposed method of modeling can be used for the optimization of parameters of the polishing process used in hard memory disk technology.

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