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STATISTICAL THEORY OF FRICTION IN INTERACTION OF A NANOPROBE WITH THE SURFACE OF A SOLID BODY

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Consideration is given to the statistical theory of friction between the probe of an atomic-force microscope and the atomically smooth surface of a solid body. Based on the calculations performed it has been inferred that the process of friction in nanocontacts is fractal. It has been shown that the fractal integro-differentiation formalism can be applied to analysis of the processes of interaction in nanocontacts.

The linear dependence of the friction force on the load (Amonton's law) is caused by the interaction and superposition of individual multiple micro- and nanocontacts of rubbing surfaces of macroscopic bodies [1]. The total area of contact of these surfaces is several orders of magnitude smaller than the nominal area. To investigate friction in nanocontacts one currently uses an atomic-force microscope operating in the regime of recording of lateral forces [2]. The device allows measurement of the forces with an accuracy of up to 10^{-12} N.

Despite certain advances made recently in "low-dimension physics," there has been no satisfactory quantitative theory of nanostructural-friction forces as yet. Thus, according to the adhesion [2] and dislocation [3] mechanisms of friction, the stick-slip sliding of a nanoprobe over the surface of a solid body is accompanied by the formation and breaking of individual interatomic bonds. In both cases, for the friction force one employs the formula

$$F = \tau S \,, \tag{1}$$

where $S = \pi R^2$. The experiments with an atomic-force microscope have shown that the sliding of a nanoprobe over the surface of a solid body is characterized in most cases by a low value of the friction force and the anomalous behavior of the friction–load dependence [2]. However it is impossible to explain these phenomena using formula (1).

In the present work, we give statistical consideration to the process of dry friction in the system probe–surface. The essence of the method is that it assumes a random character of formation and breaking of individual interatomic bonds in the process of sliding. With the use of this assumption we derive a new formula for the force of friction between the nanoprobe and the solid-body surface, which generalizes formula (1).

Let $p(S)$ be the probability of absence of interatomic bonds in the contact of area S, satisfying the condition $\lim_{S\to\infty} p(S) = 0$. As the contact area successively increases, this probability decreases so that, by virtue of statistical independence, the probability multiplication theorem will hold: $p(S + \Delta S) = p(S)p(\Delta S)$. Computing the logarithmic derivatives of this expression with respect to S, we obtain the differential equation for the unknown function $p(\Delta S)$:

$$\frac{d \ln (p\,(S + \Delta S))}{dS} = \frac{d \ln (p\,(S))}{dS} = -\,\vartheta \,. \tag{2}$$

The solution of (2) has the form

$$p\,(S) = \exp\,(-\,\vartheta S) \,. \tag{3}$$

The probability $p(S)$ must, apparently, depend on the interatomic-bond energy. In the most general form, this dependence is taken into account by the Weibull distribution [4], which is obtained from (3) at $\vartheta = \text{const}\, E^a$, where $a > 0$.

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The probability that there are interatomic bonds in the region of contact is equal to $q(S, E) = 1 - p(S, E)$. As a result, for the probability $q(S, E)$ we will have the following formula:

$$q(S, E) = 1 - p(S, E) = 1 - \exp\left(-\frac{S}{S_0}\left(\frac{E}{E_0}\right)^a\right), \tag{4}$$

where we have passed to dimensionless variables using the parameters S_0 and E_0. With account for the distribution function (4) we find the average interatomic-bond energy

$$\langle E_i\rangle = \int_0^\infty E\frac{dq(S, E)}{dE}dE = a\int_0^\infty \frac{S}{S_0}\left(\frac{E}{E_0}\right)^a \exp\left(-\frac{S}{S_0}\left(\frac{E}{E_0}\right)^a\right)dE. \tag{5}$$

Integrating (5), we obtain

$$\langle E_i\rangle = E_0\Gamma(1 + 1/a)\left(\frac{S_0}{S}\right)^{1/a}, \tag{6}$$

where $\Gamma(1 + 1/a)$ is the Euler gamma function. We note that in actual contacts we always have deformation. Its presence in no way disturbs the generality of the above considerations. Expression (6) is very simply interpreted with the use of the notion of fractal dimension [5]. As applied to our problem, the latter is introduced using the relation $N\xi^d = 1$. From this determination, we have: $N = \xi^{-d} = (R/r_a)^d$ and $d = \ln(N)/\ln(R/r_a)$ ($r_a \sim 0.1$–0.2 nm). With allowance for what has been said above, we find from (6) the average energy which must be expended in breaking the contact:

$$\langle E\rangle = \langle E_i\rangle N = E_0\Gamma(1 + d/2) = \langle E_i\rangle\left(\frac{S}{S_0}\right)^{1/a} = \langle E_i\rangle\left(\frac{R}{r_a}\right)^d, \tag{7}$$

where $d = 2/a$. The necessity of introducing the notion of fractal dimension for explanation of different experiments with an atomic-force microscope has been suggested in [3]. As the above calculations show, this is attained by using the statistical approach and the Weibull distribution, a particular case of which is a Boltzmann-type distribution with parameters $a = 1$ and $E_0 = \langle E\rangle$.

Let us calculate the force of friction between the nanoprobe and the sample. If we assume that the atoms of the rubbing bodies lose their bond when they are separated by a distance of $2r_a$ (equal to the characteristic bond length), the force to be applied to break the entire contact will be equal to $F = \langle E\rangle/2r_a$. Numerous experiments with an atomic-force microscope show that this force is not equal to zero in the absence of the external load, which is caused by the residual action of the adhesive force [2, 3]. In calculating the contact radius, the adhesive force is taken into account in the macroscopic approximation of Deryagin, Muller, and Toropov (DMT approximation) [6]. Thus, with account for (7) we obtain the following formula for the friction force:

$$F = \frac{\langle E_i\rangle}{2r_a}N = \frac{\langle E_i\rangle}{2r_a}\left(\frac{R}{r_a}\right)^d = \frac{\pi\langle E_i\rangle}{2r_a^{d+1}}\left(\frac{r_0}{K}(F_\perp + 2\pi r_0 W)\right)^{d/3}, \tag{8}$$

$$\frac{1}{K} = \frac{3}{4}\left(\frac{1 - \nu_1^2}{\mu_1} + \frac{1 - \nu_2^2}{\mu_2}\right).$$

We emphasize that the contact zone formed by the standard probe of an atomic-force microscope with a radius of curvature of the tip of tens of nanometers contains tens to hundreds of thousands of atoms. Fluctuations of the physical parameters of contact will, apparently, be small as compared to the average values of these parameters. In this case,

the use of the DMT approximation in which such macroscopic parameters as the elastic moduli and the Poisson coefficients of the probe and the sample are employed is justified.

It is quite obvious that the formula (8) obtained generalizes formula (1). It yields that with a change of unity to three in the fractal dimension of the nanocontact the exponent of the dependence friction force–load changes from 1/3 to 1, which explains all the available contradictory experimental results [2]. Thus, the power dependence of the friction force on the load with exponents of 0.1 to 0.3 is revealed in computer modeling of the interaction of open single-layer nanontubes with a (100)-type diamond face [7]. Within the framework of the model in question, this corresponds to the fractal dimension $d \le 1$. In the case of a regular two-dimensional contact (d = 2), expression (8) precisely yields formula (4.4) from [2] and formula (4) from [5], which describe hard contacts. If spatially three-dimensional structures (solid atomic clusters) are formed due to the wear, chemical reactions, or phase transformations in the region of contact, then $d \to 3$ and the corresponding dependence friction–load becomes linear. Such a situation, for example, has been observed in atomic-force microscopic experiments on alkali halide crystals [2]. Furthermore, it is pertinent to note here that friction at the macroscopic level, when the dependence of the friction force on the load is nearly linear, results in the formation of fractal surfaces with a dimension of $d > 2$ [8].

In the present work, we have noted a very interesting fact. It was shown that expression (7) can be obtained with the use of the fractional integro-differential formalism, i.e., the mathematical apparatus widely used in the fractal theory. We demonstrate this conclusion, employing the notion of surface energy γ. In accordance with thermodynamic determination, we have

$$\gamma = \frac{dG}{dS} = \frac{1}{S_0}\frac{dG}{d\Omega}, \tag{9}$$

where $\Omega = S/S_0$. Employing the composition law for a fractional derivative [9, 10], we can rewrite formula (9) as follows:

$$\gamma S_0 = D_{0\Omega}^{1/a} E_0, \tag{10}$$

where

$$D_{0\Omega}^{1/a} E_0 = \frac{1}{\Gamma(1 + [1/a] - 1/a)} \frac{d^{[1/a]+1}}{d\Omega^{[1/a]+1}} \int_0^{\Omega} \frac{E_0 d\Omega'}{(\Omega - \Omega')^{1/a-[1/a]}}, \quad E_0 = D_{0\Omega}^{1-1/a} G.$$

Here $D_{0\Omega}^{m}$ is the operator of fractional differentiation of Riemann and Liouville of order n, while the square brackets denote the integral part of the number. Since the surface energy γ is independent of Ω (which follows from physical considerations), the function represented in the form

$$E_0 = \frac{\gamma S_0}{\Gamma(1 + 1/a)} \Omega^{1/a}, \tag{11}$$

will be the solution of Eq. (10). Formula (11) yields the expression for the average energy of breaking of the contact:

$$\langle E \rangle = E_0 \Gamma(1 + 1/a) = \gamma S_0 \Omega^{1/a} = \gamma S_0 \left(\frac{S}{S_0}\right)^{1/a} = \langle E_i \rangle \left(\frac{R}{r_a}\right)^{2/a}, \tag{12}$$

where $S = \pi R^2$, $S_0 = \pi r_a^2$, and $\langle E_i \rangle = \gamma \pi r_a^2$. It can be seen that the obtained formula (12) coincides with (7) for $a = 2/d$. The correspondence between the statistical approach and the approach based on the fractional integro-differentiation formalism comes as no surprise, in principle. In particular, it is well known [9] that the function $p(S, E)$ (Weibull distribution) determined by expression (3) is closely related to the solutions of different differential equations of fractional order. Thus, we can draw the following important conclusion: the use of fractional integro-differentiation is mathematically equivalent to the passage from the thermodynamic description of a system to a statistical description.

NOTATION

r_0, radius of curvature of the tip of the probe; F, friction force; $F_\perp$, load; W, specific energy of adhesion of flat surfaces; $\mu_{1,2}$, elastic moduli of the probe and the sample; $\nu_{1,2}$, Poisson coefficient; G, Gibbs thermodynamic potential; Ω, dimensionless contact area; d, fractal dimension of the contact; r_a, reduced atomic radius; τ, tangential stress; S, contact area; R, contact radius; γ, surface energy; E, interatomic-bond energy; $\langle E_i \rangle$, average interatomic-bond energy; $\langle E \rangle$, average energy of breaking of the contact; ξ, similarity parameter; $p(S)$, probability of absence of interatomic bonds in the region of contact; $q(S)$, probability of presence of interatomic bonds in the region of contact; ϑ, positive constant; Γ, Euler gamma function; N, number of interatomic bonds in the region of contact; K, reduced elastic module; S_0, E_0, and a, parameters of the Weibull distribution. Subscripts: a, atomic; i, individual interatomic bond; m, order of a fractional derivative; 0, parameters of the Weibull distribution.

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