

Nonlinear model of nanocontact friction in atomic force microscopy

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The paper proposes an analytical model for the AFM spherical tip friction against a solid surface, which accounts for the formation of a deformable finitethickness interlayer in the contact region. The interlayer's mechanical response is described by a generalized Hooke's law. A power-law friction force dependence on the normal load is obtained; the exponent is determined by nonlinearity of the contact-region mechanical response. The model demonstrates a good agreement with experimental data and explains the wide-range variations in the exponent.

Keywords: nanotribology, nanocontact, nonlinear elasticity, friction force, power law, atomic force microscopy.

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Theoretical description of nanofriction is based on analytical models by Hertz, Johnson–Kendall–Roberts, Derjaguin–Muller–Toporov, and Magis–Dugdale [1,2] that are widely used to interpret experiments in atomic force microscopy (AFM). These models interrelate the friction force with load force and materials' elastic properties, but do not directly account for the atomic structure, contact discreteness, and complex mechanisms for deformation and wear. Significant evolution in this field is associated with applying the molecular dynamics (MD) method [3–8]. It is used to analyze nanoindentation and sliding and investigate the role of dislocations and phase transformations, as well as the adhesion–sliding mode. In addition, the MD method enables examining the influence of load, speed, temperature, and geometry of the contact. Nevertheless, as shown by the collected experimental data, neither analytical contact models nor available numerical approaches provide a universal explanation of the observed effects. For instance, in the nanocontacts there have been revealed the power-law friction force dependences on vertical-load force of the $F_L \propto F_N^\beta$ type, where index β widely ranges from 0.3 to 1 depending on the material, contact geometry and external conditions.

Paper [9] has proposed a dislocation-based mechanism for nanofriction which implies that, in scanning an atomically smooth surface, the contact region is interpreted as an edge dislocation loop covering the region of the probe-surface interaction. This model provided dependence $F_L \propto F_N^{2/3}$. It is argued for by similarity of the adhesion–sliding effect to the jumping motion of dislocations with the Burgers vector, minimal tangential stresses in sliding over densely packed planes, formation of the „bad crystal region“ in MD-modeling, and correlation between the probe acceleration and acoustic emission. However, further research has shown that under real conditions the contact region comprises hundreds to thousands of atoms and gets formed as a result of a complex combination of adhesive, elastic,

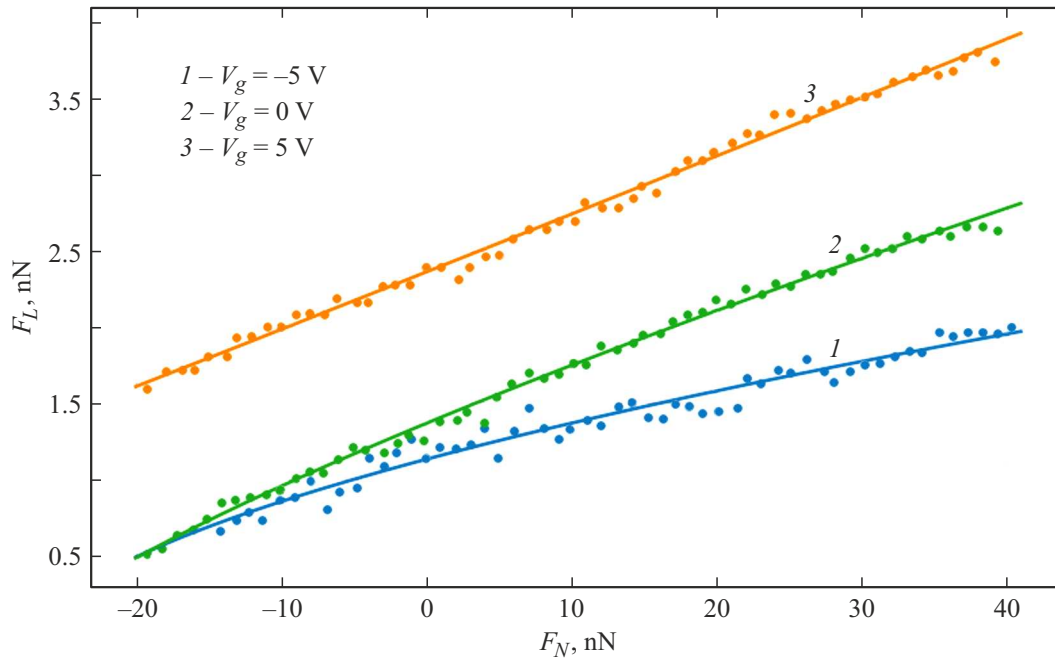
and electronic interactions. In addition, in the case of dislocation-based interpretation of the contact boundary, certain difficulties arise in quantitative comparison with experimental data exhibiting variations in index β . This indicates a complex nature of nanofriction where the contribution of deformation, adhesion, and, in some cases, capillary effects significantly depends on the specific tribosystem; this makes insufficient the universal description with only the dislocation mechanism.

In this study, the hypothesis of [9] has been reinterpreted: the region of the probe-sample contact is considered as a special „effective interlayer“ where local atomic rearrangements and partial plasticity take place. Mechanical behavior of this interlayer is described by a more general power law [10,11], which qualitatively complies with the well-known Ogden's model [12,13] and molecular dynamics data [3–8,14–17]. The latter show that in the contact region there emerges a disordered defective structure capable of almost reversible nonlinear deformations. This approach enables accounting for the local contact nonlinearity under the conditions of quasi-static sliding.

In the case of an isotropic nonlinear material of the contact interlayer, the relationship between normal stress σ_{zz} and relative compression strain ε_{zz} is given by ratio

$$\sigma_{zz} = E(\varepsilon_{zz})^\alpha, \quad (1)$$

where E is the effective elasticity modulus, α is the nonlinearity index. When $\alpha = 1$, ratio (1) transforms into the Hooke's law; when $\alpha = 0$, it describes an ideal plastic flow with a constant yield stress. In the classical models [1,2], elastic properties of the contact are assumed to be the same as of the material as a whole. However, this is not enough to explain the experimental data on nanofriction. Therefore, it is necessary to consider the contact region as an area with its own characteristics; for this purpose, its effective thickness δ_0 is introduced. For the vertical



Friction force of the AFM Si-probe contacting the MoS₂ monolayer on the SiO₂/Si substrate as a function of load at different stresses. Parameters F_A and β are, respectively: 1 — 26.4 nN and 0.6; 2 — 27.2 nN and 0.8; 3 — 65.0 nN and 1.0.

deformation, obtain:

$$\varepsilon_{zz}(r) \approx \frac{\delta - r^2/(2R)}{\delta_0}, \quad (2)$$

where δ is the probe penetration depth, r is the radial coordinate in the contact plane, R is the probe tip curvature radius. Relation (2) implies that vertical deformation is localized in the terminating layer and is defined as the ratio of surface convergences to this layer thickness at $\delta - r^2/(2R) \geq 0$ and $\delta \lesssim \delta_0$. The probe's normal force is determined by integrating stress over the contact area

$$F_N = 2\pi \int_0^a \sigma_{zz}(r) r dr = \frac{2\pi E}{\delta_0^\alpha} \int_0^a \left(\delta - \frac{r^2}{2R} \right)^\alpha r dr, \quad (3)$$

where a is the contact region radius. Using variable substitutions $r^2 = 2R\delta s$ and $r dr = R\delta ds$, transform (3) to

$$F_N = \frac{2\pi R E \delta^{\alpha+1}}{\delta_0^\alpha} \int_0^1 (1-s)^\alpha ds = \frac{2\pi R E}{\alpha+1} \frac{\delta^{\alpha+1}}{\delta_0^\alpha}. \quad (4)$$

In the spherical geometry, contact area is $A = \pi a^2 = 2\pi R\delta$; static friction force according to the Bowden–Tabor formula [18] is proportional to this area:

$$F_L = \tau A = 2\pi R\delta\tau, \quad (5)$$

where τ is the effective tangential shear stress in the contact region, which is weakly dependent on the load. Excluding

δ from (4) and (5), obtain

$$F_L = 2\pi R\delta_0\tau \left[\frac{(\alpha+1)(F_\perp + F_A)}{2\pi R\delta_0 E} \right]^\beta, \quad (6)$$

where $\beta = 1/(\alpha+1)$, and relation $F_N = F_\perp + F_A$ is taken into account ($F_\perp$ is the external load acting on the probe, $F_A > 0$ is the adhesion-induced force of pressing the probe against the sample). Thus, the power-law dependence of the friction force on load arises naturally from the nonlinear mechanical response of the contact region and from spherical contact geometry.

To verify formula (6), a comparison with experimental data from [19] was performed; the result is shown in the figure. In the experiments, the dependence of the AFM silicon probe friction force on the load on the surface of the MoS₂ monolayer applied on the SiO₂/Si substrate was studied at different probe-sample voltages V_g . The data from [19] were chosen because they exhibit the power index β variation from ~ 0.5 to ~ 1 with varying V_g , which cannot be explained by classical contact models with fixed β . Errors in determining parameters β and F_A are 4–16%, while determination coefficient R^2 ranges from 0.960 to 0.995; this evidences a good agreement between the model and experiment. When the loads are tens of nanonewtons and applied voltage amounts to 5 V, the contact region obviously includes not only the probe tip and MoS₂ monolayer, but also the SiO₂/Si substrate part involved in deformation and friction. Within the proposed model, the curves' shift along the load axis is interpreted as variation in adhesive force F_A , while the slope variation is interpreted as variation in parameter α that characterizes

the contact region nonlinearity. This phenomenological model does not consider the microscopic mechanism of the electric field impact (variations in adhesion, charge screening, electron-phonon dissipation). We may only note that simultaneous variations in F_A and β with changing voltage polarity demonstrates a close relationship between the electronic and mechanical properties of the contact interlayer; accumulation or depletion of charge carriers modifies both the interatomic interaction strength and nonlinear rigidity of the contact.

Note that the special case at $\beta = 1/2$ ($\alpha = 1$) corresponds to a linear-elastic response of the interlayer material; this is consistent with the limit of small deformations in nonlinear elasticity models [10–13]. Another special case $\beta = 2/3$ ($\alpha = 1/2$) formally reproduces the power index in the classical Hertz theory [1,2], however, in the model under consideration it arises due to not the half-space geometry but nonlinearity of the interlayer material. This emphasizes that identical friction force power-law dependences on the load may be realized in various physical processes occurring in the nanocontact. Here we should also note that MD simulation of nanocontacts exhibits systematic deviations from the Hertz theory [14–17]. The deformation is localized in a near-surface region with a finite thickness of about several interatomic distances and is characterized by the presence of an internal scale parameter similar to parameter δ_0 introduced in this work. In this regard, using δ_0 instead of an infinite half-space in the Hertz theory seems to be a more adequate description of nanocontact physics.

What is important is that definitive relation (1) does not impose restrictions on the deformation reversibility. In continuum mechanics, power laws are used to describe both physically nonlinear elastic materials (within Ogden-type models [12,13]) and plastic flows with strain hardening. In the latter case, parameter α corresponds to the hardening power, while at $\alpha = 0$ the model degenerates into the case of ideal plasticity ($\sigma = \text{const}$) which gives a linear friction force dependence on load ($\beta = 1$). Thus, the proposed model is not rigidly linked to a specific physical mechanism of deformation (elastic or plastic) but, in essence, describes a general class of problems in which local response the contact-region material obeys a power law.

Concerning this study, we have made the following conclusions. A theoretical model of the AFM probe friction against the solid body surface has been developed; the model involves the nonlinear mechanical contact-region response and adhesive interactions. Dissipative processes are not described explicitly but are parameterized through effective tangential stress τ , which meets the standard approach [1,2]. The model provides a unified description of the observed power-law dependences of friction force on load and is applicable in the steady-state sliding mode.

Conflict of interests

The author declares that he has no conflict of interests.

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