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MISCELLANEA

MODEL OF MOTION OF THE PROBE OF AN ATOMIC-FORCE MICROSCOPE IN THE SEMICONTACT REGIME

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The equation of motion of the oscillating probe of an atomic-force microscope in the field of surface forces of an elastic sample was numerically solved. The influence of the position of the probe and the elastic modulus of the sample on the dynamic parameters of the probe motion and the characteristics of the contact deformation of the sample was estimated.

Introduction. The formation of an image in scanning probe microscopy and, in particular, in atomic-force microscopy (AFM) is based on the control of the parameters of the mechanical motion of a micromechanical probe, consisting of a microcantilever with a microindenter set at its free end, near the surface of a sample [1, 2]. The bending of the cantilever of such a probe in the process of its contact with the surface of a sample (contact regime) and the change in the parameters of the oscillations of the cantilever (semicontact dynamic regime) are determined to a large extent by the contact interaction of the microindenter with the surface of the sample [1]. In the case where a topographic 3D image of a region of a sample is formed with the use of a scanning probe, the force of interaction of the probe indenter with the sample (contact regime) or the gradient of this force (dynamic regime) is held constant in the process of scanning with the use of an electron-feedback system [3, 4]. The local mechanical properties of the material of the surface nanolayers of a sample can be estimated by increasing the load at the site of contact of the indenter of a probe with the sample and by deforming nanometer areas of its surface [5, 6]. This procedure is called static force spectroscopy [5, 7] and is effectively used in the nanoindentation of materials with the use of an atomic-force microscope. The procedure of dynamic force spectroscopy, in which the cantilever of a probe executes resonance oscillations when the probe approaches the surface of a sample, is no less informative [2]. The decrease in the amplitude of these oscillations and shift of their frequency and phase in the process of interaction of the oscillating-probe indenter with the surface of the sample depend on the viscoelastic and adhesive properties of its surface. However, since many factors influence the motion of a microprobe in the field of surface forces of a sample under conditions of deformation of its surface layers, it is difficult to determine the functional relation between the dynamic parameters of the probe and the characteristics of the material of the sample. Therefore, this problem has not yet been uniquely solved [2].

In the present work, a numerical simulation of the motion of the oscillating probe of an atomic-force microscope near the surface of a sample has been performed and the dependence of the deformation of the material of the surface layers of the sample on the distance between it and the probe and the elastic properties of the sample has been analyzed for the purpose of constructing an adequate description of the procedure of dynamic force spectroscopy and using it for characterizing materials in a nanoscale.

Formulation of the Problem and Computational Model. Forced oscillations of a microscopic cantilever with an indenter set at its free end are considered. The cantilever indenter is located at a distance z_{pos} from the horizontal surface of the sample (Fig. 1). The driving force, under the action of which the cantilever begins to oscillate, changes by the harmonic law. This force is applied at the point of fixation of the beam-cantilever (the amplitude of

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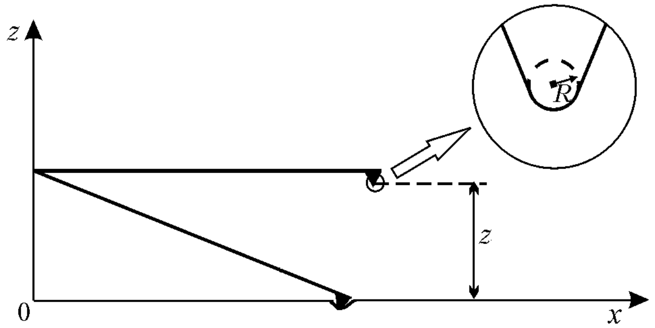

Fig. 1. Probe-cantilever system in the semicontact regime of operation of an atomic-force microscope.

oscillations at the fixation point is a_{bim} and their frequency is ω). The Young modulus and the Poisson coefficients of the sample and the cantilever indenter are, respectively, E_1 and ν_1 and E_2 and ν_2.

In the description of the motion of a cantilever with an indenter, a vertically fixed spring of rigidity k (equivalent to the flexural rigidity of the cantilever) with a stationary top point is usually used instead of the oscillating cantilever, and an oscillating point mass m concentrated at the free end of the spring is used instead of the cantilever indenter. The working (contacting) part of the indenter is simulated by a spherical segment with a curvature of radius R. It is assumed that the quality factor of the oscillating system is Q and the frequency of natural oscillations of the spring with an indenter is ω_0.

Since the geometric dimensions and the mass of the oscillator being considered are small, the field of surface forces in the clearance between the probe indenter and the sample acts on the indenter and has a profound impact on the motion of the probe. Moreover, in every cycle of steady-state oscillations of the probe, the probe indenter comes, at the lower point of its motion, in contact with the sample, with the result that the contacting bodies are subjected to an elastic deformation. The inclusion of the elastic reaction of the sample and the interactions realized due to the off-contact surface forces introduces a nonlinearity into the equation of motion of the probe cantilever. The force applied to the indenter and the character of oscillations of the cantilever are determined to a large extent by the distance between the indenter and the surface of the sample; this distance, in turn, is determined by the position of the probe relative to the surface of the sample z_{pos} and the amplitude of oscillations of the free end of the cantilever. For example, the indenter cannot come in contact with the surface of a sample and can interact with its surface only due to the Van der Waals surface forces. The opposite situation is realized in the case where the indenter oscillates as a result of its contact with the surface of the sample.

In the present work, the general case of semicontact oscillations is considered. The indenter moves in the field of the attracting surface forces of a sample and, when it comes in contact with the surface of the sample, is subjected to the action of the repulsive contact forces. The forces of interaction of the indenter with the surface of the sample can be calculated with the use of the model proposed, e.g., in [8]. In this model, the molecular-nature surface forces (Van der Waals forces) are assumed to be dependent on the value of the clearance separating the indenter of a probe and the surface of a sample and are calculated as a derivative of the Lennard-Jones potential:

$$F_{\text{att}}(z) = -\frac{HR}{6\sigma}\frac{\partial}{\partial z}\left(\frac{1}{210}\left(\frac{\sigma}{z}\right)^7 - \frac{\sigma}{z}\right). \tag{1}$$

The repulsive force arising as a result of the elastic deformation of the material of a sample was determined by the following relation for the contact of a sphere with a plane from the Hertz theory:

$$F_{\text{rep}}(z) = k_s R^{1/2}(-d^{3/2}). \tag{2}$$

Here

$$k_{\mathrm{s}} = \frac{4}{3\pi}\frac{1}{\kappa_{\mathrm{eff}}} = \frac{4}{3\pi}\frac{1}{\kappa_1 + \kappa_2}\,; \quad \kappa_i = \frac{1 - \nu_i^2}{\pi E_i}\,, \quad i = \overline{1, 2}\,; \quad d = z - z_{F_0}\,.$$

In this case, the system of equations for the oscillations of a spring with an indenter will have the form

$$\begin{aligned} &m\frac{\partial^2 z}{\partial t^2} + \frac{m\omega_0}{Q}\frac{\partial z}{\partial t} + kz = kz_{\mathrm{pos}} + a_{\mathrm{bim}}\,k\sin(\omega t) - \frac{HR}{6}\left(\frac{1}{z^2} - \frac{\sigma^6}{30z^8}\right), \quad z > z_{F_0}\,; \\ &m\frac{\partial^2 z}{\partial t^2} + \frac{m\omega_0}{Q}\frac{\partial z}{\partial t} + kz = kz_{\mathrm{pos}} + a_{\mathrm{bim}}\,k\sin(\omega t) + k_{\mathrm{s}}R^{1/2}\left(z_{F_0} - z\right)^{3/2}, \quad z \le z_{F_0}\,. \end{aligned} \tag{3}$$

This system is solved at the following initial conditions:

$$z\big|_{t=0} = z_{\mathrm{pos}}\,; \quad \left.\frac{\partial z}{\partial t}\right|_{t=0} = 0\,.$$

For the program realization, the system of second-order differential equations (3) was rearranged to a system of first-order differential equations. For this purpose, we introduced new variables: $x_1 = z$ and $x_2 = \partial z/\partial t$. Since $k/m = \omega_0^2$, system (3) takes the form

$$\frac{\partial x_1}{\partial t} = x_2\,;$$

$$\begin{aligned} &\frac{\partial x_2}{\partial t} + \frac{\omega_0}{Q}x_2 + \omega_0^2 x_1 = \omega_0^2 z_{\mathrm{pos}} + a_{\mathrm{bim}}\omega_0^2\sin(\omega t) - \frac{HR\omega_0^2}{6k}\left(\frac{1}{x_1^2} - \frac{\sigma^6}{30x_1^8}\right), \quad x_1 > z_{F_0}\,; \\ &\frac{\partial x_2}{\partial t} + \frac{\omega_0}{Q}x_2 + \omega_0^2 x_1 = \omega_0^2 z_{\mathrm{pos}} + a_{\mathrm{bim}}\omega_0^2\sin(\omega t) + \frac{k_{\mathrm{s}}R^{1/2}\omega_0^2}{k}\left(z_{F_0} - x_1\right)^{3/2}, \quad x_1 \le z_{F_0}\,. \end{aligned} \tag{4}$$

The numerical simulation of the process of oscillations of the probe of an atomic-force microscope was performed using the Mathematica package [8]. A solution of the above system of equations was obtained in the form of interpolation functions.

The mechanical behavior of the probe–sample system depends on the initial parameters, which can be conditionally divided into three groups: 1) the parameters characterizing the microprobe (resonance frequency, quality factor, rigidity of the cantilever, radius of the indenter curvature, Young modulus, Poisson coefficients of the material and the indenter); 2) the parameters determined by the AFM operator (amplitude of free oscillations of the cantilever, position of the probe relative to the sample); 3) the parameters of the material of the sample (Hamaker constant, interatomic distance, Young modulus, Poisson coefficients of the material of the sample). The frequency of the driving force will be assumed to be equal to $\omega = \omega_0$, which does not decrease the generality of the description. This choice of the working frequency corresponds to the situation arising frequently in practice because, in dynamic atomic-force microscopy, measurements are usually carried out in the resonance regime or at a frequency close to the resonance frequency [2, 8, 9].

Results of the Computational Experiment and Their Discussion. A numerical experiment has been carried out to investigate the possibility of control of the motion of the indenter of the probe of an atomic-force microscope and to determine the features of the deformation of the surface layers of a sample by the probe indenter in the dynamic regime of operation of the microscope. The determination of the relation between the oscillations of the probe and the mechanical properties of the material of a sample is of practical importance for the development of methods of dynamic nanoindention. To obtain this relation, we investigated the time dependence of the coordinate z of the

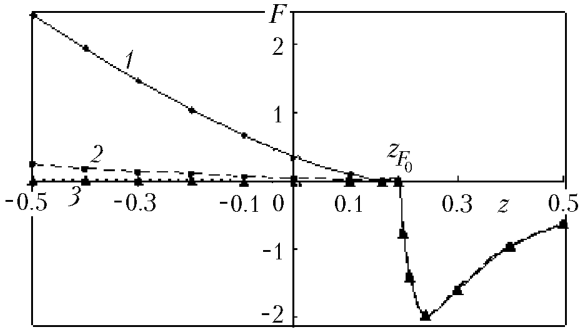

Fig. 2. Dependence of the force of interaction of the probe with the surfaces of three different samples on the distance between the probe and the samples: $E = 1$ (1), 0.1 (2), and 0.01 GPa (3). z, nm; F, nN.

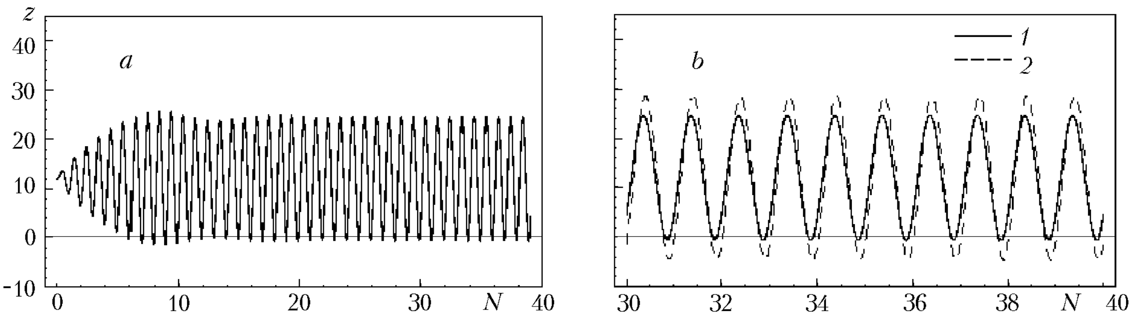

Fig. 3. Development of oscillations of a microcantilever: a) motion of the cantilever indenter beginning with the instant a driving force is applied and ending at the 40th oscillation cycle; b) motion of the cantilever in the case of steady-state oscillations [1) oscillations of the indenter in the process of its interaction with the surface of a sample; 2) oscillations of the indenter in the absence of the sample]. z, nm.

probe of an atomic-force microscope or the number of its oscillation cycles as well as the dependence of the rate of motion of the indenter of the probe on the coordinate of its position, determining the depth of penetration of the probe into the surface of the sample and the force of elastic repulsion of the indenter by the sample. Varying the initial parameters of the oscillating system, we determined the dependence of the amplitude and phase of oscillations of the indenter, the deformation of the sample, the radius and time of contact of the indenter with the sample, the load on the sample, and the repulsive force on the properties of the material of the sample.

Samples with elastic moduli of 0.01, 0.1, and 1 GPa were investigated. This range of elastic properties corresponds to the materials, polymers for the most part, for which AFM nanoindention can be performed with the use of commercial silicon microprobes. We constructed numerical dependences defining the motion of the probe interacting with the above-indicated samples (Figs. 2–5). The following model parameters were used in the computational experiment: $k = 10$ N/m, $f = \omega/(2\pi) = f_0 = 100$ kHz, $R = 10$ nm, $E_2 = 179$ GPa (corresponds to silicon), $\nu_1 = \nu_2 = 0.3$, $H = 0.1$ mN·nm, $\sigma = 0.34$ nm, $a_{\text{bim}} = 0.8$ nm. The quality factor of the system Q was assumed to be equal to 100.

Figure 2 shows the dependence of the force of interaction of the probe indenter with a sample on the distance between them. It is seen that the repulsive force (the curves to the left of the point z_{F_0}) increases with increase in the elastic modulus of the material. In the calculations, the surface energy of the samples was assumed to be constant; therefore, the attracting force (the curves to the right of the point z_{F_0}) remains unchanged. Such dependences are used below for simulation of the dynamics of the probe in the semicontact regime.

The development of the oscillations of the probe with time beginning with the instant a driving force is applied to it is shown in Fig. 3. It is seen that the oscillation process is gradually established when the frequency of the

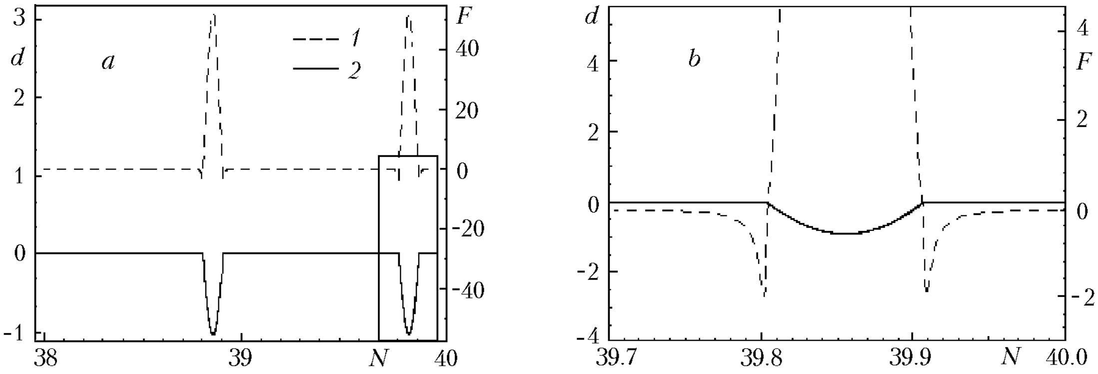

Fig. 4. Force of interaction of the probe indenter with a sample (1) and deformation of the sample (2) within two cycles of oscillations (a) and within one-half an oscillation cycle (b). F, nN; d, nm.

driving force becomes equal to the resonance frequency of the probe. The zero level in the graph corresponds to the level of the surface of a sample. It is known that the main parameter influencing the stabilization time of oscillations of a system, i.e., the number of its oscillation cycles for which the oscillations become stationary, is the quality factor Q of this system. In the case considered (for Q = 20 and E_1 = 10 GPa), the oscillations of the probe become stationary at the 40th oscillation cycle. It should be noted that the surface of a sample does not influence the symmetry of oscillations of the probe relative to the position z_{pos} (Fig. 3a, curve 1 in Fig. 3b); however, the amplitude of its oscillations in the semicontact regime is smaller as compared to the amplitude of the free oscillations (Fig. 3b, curve 2).

We now will analyze the action of the probe indenter on a sample in the case of its local contact deformation. Figure 4 shows the changes in the deformation of the sample and in the force of interaction of it with the probe. In Fig. 4a, two cycles of oscillations of the probe are shown, and, for a more comprehensive analysis, Fig. 4b shows the part of an oscillation cycle of the probe for which the indenter makes contact with a sample at $z_{\text{pos}} \approx A_0$. On the curve of the interaction force (curve 1) there are spikes caused by the attracting force acting at the beginning and at the end of the contact stage. For the initial model parameters selected, the repulsive forces dominate over the Van der Waals attracting forces throughout the oscillation cycle of the probe. The contact time comprises an insignificant part of the oscillation period (Fig. 4a); for the largest part of this period, the indenter is at a distance from the surface of the sample, at which the forces of action of the sample on the indenter are close to zero. These results are close to the results obtained in [4].

Figure 5 shows dependences constructed for the case where the probe approaches samples under identical conditions. These dependences demonstrate the influence of the elastic modulus of a sample on the following characteristics of oscillations and interaction of the indenter with the sample: the amplitude of oscillations of the probe, the maximum force of interaction of the probe with the sample, the time of contact of the probe with the sample for one oscillation cycle, and the depth of deformation of the sample. In this case, the position of the probe z_{pos} was changed from 84 nm to 0. The amplitude of forced oscillations of the probe away from the surface of the sample (free oscillations) was assumed to be equal to A_0 = 82.3 nm in all cases. At a distance larger than A_0, the probe does not come in contact with the surface of the sample. It is seen from Fig. 5a that the amplitude of oscillations of the probe decreases with decrease in z_{pos}, i.e., as it approaches the sample. The gradient of change in this amplitude increases with increase in the elastic modulus of the sample. In the case where the probe interacts with more rigid samples, the amplitude of its oscillations decreases more rapidly. In Fig. 5b, the calculated values of the maximum force acting on the probe indenter are presented. In the range of distances z_{pos} being considered, the attracting forces prevail; these forces increase with increase in the Young modulus of the material of a sample; negative (attracting) interaction forces can arise only in the region where $z_{\text{pos}} > 82$ nm. In the region of initial contacts ($z_{\text{pos}} \approx A_0$), the Van der Waals forces contribute significantly to the average force of interaction of the probe indenter with the surface of the sample. Since the repulsive force is larger in the case of interaction of the probe with softer samples, the attracting interactions make a large contribution to the total interaction force. The contact time increases (Fig. 5c) when the probe indenter approaches a sample. At small values of z_{pos}, the difference between the times of contact with different materials is

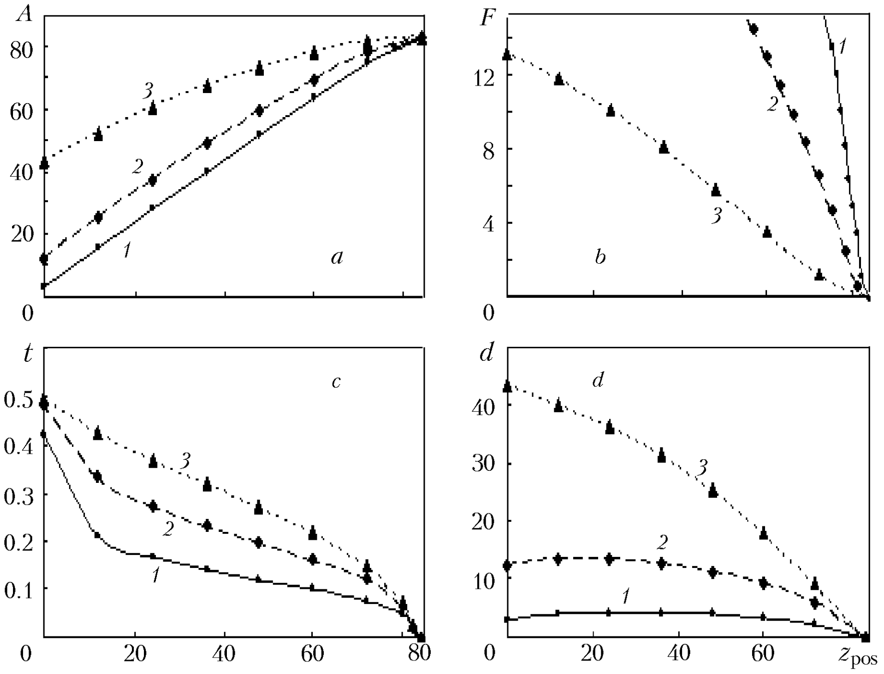

Fig. 5. Dependences of the amplitude of oscillations of the probe (a), the maximum force of interaction of the probe indenter with a sample (b), the time of contact of the probe with the sample (c), and the maximum depth of deformation of the sample (d) on the distance z_{pos}, obtained for different materials: E = 1 (1), 0.1 (2), 0.01 GPa (3). z_{pos}, d, A, nm; F, nN; t, sec.

small and is close to half the period of oscillations of the probe. Comparison of Figs. 5d and 5c shows that, when the contact time is small, more rigid materials experience a smaller deformation; in the case where z_{pos} is close to zero, the amplitude of oscillations of the probe is practically equal to zero (Fig. 5a). For softer samples, the amplitude of oscillations of the probe near their surface ($z_{pos} = 0$) is two times smaller than its initial oscillation amplitude. In this case, the deformation of the sample and the time of contact of the probe with it are large. The dependences shown in Fig. 5 are similar in character to the results of analogous investigations performed in [5], despite the fact that a different range of Young moduli was used in the indicated work for simulation of samples.

A similar numerical analysis was performed in [10, 11]. The contact times, presented in Fig. 5c, agree well with the results obtained in [11, 12]: even for the softest materials and for small distances z_{pos} between the probe and the surface of the samples, the contact time does not exeed the half-period of oscillations of the probe.

In the case where the surface of a sample is moved relative to the point of fixation of the probe of an atomic-force microscope, with which the scanning of the sample is carried out (for example, a vertical approach–removal in the process of dynamic indention or a motion in the process of scanning), the time of movement from one measurement point to another should be not smaller than the time of establishment of a stable regime; this time is usually equal to 0.3–20 msec. The time of movement of the probe between two neighboring measurement points should be not smaller than the indicated time.

When an atomic-force microscope works in a semicontact regime, the force of interaction of the indenter of its probe with the surface of the sample influences the operation of the microscope, which introduces nonlinear effects into the dynamics of motion of the probe and makes the obtaining of an analytical solution defining the motion of the probe indenter impossible. Therefore, the oscillations of the probe of an atomic-force microscope should be investigated with the use of numerical models that allow one to describe the motion of the probe and the contact interaction in the probe–sample system as well as to estimate the influence of different parameters of the probe on its oscillations.

The consistency of the results obtained by us and their agreement with the analogous data obtained by other authors (e.g., in [8]) allows the conclusion that the Hertz contact model combined with noncontact forces changing by the Lennard-Jones law and the approach described in the present work can be used for investigating the work of the system being considered under various conditions. Using the model proposed, one can analyze the influence of the oscillations of the probe of an atomic-force microscope and its characteristics on the contact of the probe indenter with a sample and, on the other hand, the influence of different parameters of the interaction of this indenter with the sample on the oscillations of the probe–sample system. This makes it possible to give practical recommendations on the use of any parameters of the probe of an atomic-force microscope, including the determined parameters of its oscillations, in investigating different samples.

The possibility of approximation of a continuous beam by a spring of point mass was considered in [13]. In [1], it was shown that for the most typical condition of work of an atomic-force microscope (in air), the approximation of the cantilever of its probe by a spring in calculations gives a fairly exact description of the motion of the probe, even though it is recommended by the authors of this work to use, in this case, small amplitudes of oscillations of the probe (smaller than 30 nm). At the same time, they present the results of calculations carried out with the use of this approximation at larger oscillation amplitudes (60–100 nm) [10, 11]. We used this range in our calculations.

Conclusions. In the present work, a numerical simulation of the motion of the probe of an atomic-force microscope interacting with the surface of a sample has been performed. The results obtained allow one to investigate such important characteristics of the work of an atomic-force microscope as the amplitude of oscillations of its probe, the force of interaction of the probe indenter with a sample, the time of contact of the indenter with the sample, and the deformation of the sample. The deformation of samples with different elastic moduli was estimated and the amplitude of oscillations of the probe and the time of its contact with the sample were calculated. The dependences obtained are of practical importance and can be used for interpretating the results of investigations of the surface of a sample in the semicontact regime of atomic-force microscopy and dynamic force spectroscopy in the procedure of nanoindention.

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NOTATION

A, working amplitude of oscillations of the indenter of a probe, nm; A_0, amplitude of free oscillations of the indenter outside the field of action of the surface forces of a sample, nm; a_{bim}, amplitude of the harmonic force, nm; d, depth of penetration of the indenter into the surface of the sample, nm; E, equivalent Young modulus, Pa; E_1 and E_2, Young moduli of the sample and the indenter, Pa; $F(x, t)$, all forces acting on a unit length of the indenter, nN/nm; $F_{\text{att}}(z)$, long-range attracting forces, nN; $F_{\text{rep}}(z)$, short-range repulsive forces, nN; H, Hamaker constant, nN·nm; k, rigidity of the probe cantilever, N/m; k_s, reduced rigidity of the system, N/m; m, mass of the probe cantilever with an indenter, kg; N, number of a cycle; R, radius of curvature of the indenter, nm; t, time, sec; Q, quality factor of the cantilever; z, position of the indenter, nm; z_{F_0}, distance at which the expression for the Lennard-Jones force turns to zero, nm; z_{pos}, the position of the point of fixation of the cantilever above the surface of the sample, nm; ν_1 and ν_2, Poisson coefficients of the sample and the indenter; σ, interatomic distance, nm; ω, angular frequency of the harmonic force, Hz; ω_0, angular eigenfrequency of the cantilever, Hz. Subscripts: bim, biharmonic piezoelectric element; att, attraction; rep, repulsion; s, system; pos, position; eff, effective.

REFERENCES

1. H. J. Butt, B. Cappella, and M. Kappl, Force measurements with the atomic force microscope: Technique, interpretation and applications, *Surface Sci. Rep.*, **59**, 1–152 (2005).
2. R. García and P. Pérez, Dynamic atomic microscopy methods, *Surface Sci. Rep.*, **47**, 197–301 (2002).
3. V. L. Mironov, *Principles of Scanning-Probe Microscopy* [in Russian], Tekhnosfera, Moscow (2004).
4. D. Sarid, *Scanning Probe Microscopy with Applications to Electric*, *Magnetic and Atomic Forces*, Oxford University Press, New York (1994).
5. A. C. Fischer-Cripps, *Nanoindentation*, Springer-Verlag, New York (2004).

6. S. A. Chizhik, Z. Huang, V. V. Gorbunov, N. K. Myshkin, and V. V. Tsukruk, Micromechanical properties of elastic polymeric materials as probed by scanning force microscopy, *Langmuir*, **14**, 2606–2609 (1998).
7. M. Salerno and I. Bykov, Tutorial: Mapping adhesion forces and calculating elasticity in contact-mode AFM, *Microscopy Analysis*, **20**, No. 2, 5–8 (2006).
8. D. Sarid, *Exploring Scanning Probe Microscopy with Mathematica*, John Wiley & Sons, Inc., New York (1997).
9. D. Sarid, T. G. Ruskell, R. K. Workman, and D. Chen, Driven nonlinear atomic force microscopy cantilevers: From noncontact to tapping modes of operation, *J. Vacuum Sci. Technol.*, **14**, No. 2, 864–867 (1996).
10. A. San Paulo and R. García, Amplitude, deformation and phase shift in amplitude modulation atomic force microscopy: A numerical study for compliant materials, *Surface Sci.*, **471**, 71–79 (2001).
11. J. Tamayo and R. García, Deformation, contact time, and phase contrast in tapping mode scanning force microscopy, *Langmuir*, **12**, No. 18, 4430–4435 (1996).
12. A. Ulcinas and V. Snitka, Intermittent contact AFM using the higher modes of weak cantilever, *Ultramicroscopy*, **86**, 217–222 (2001).
13. T. R. Rodriguez and R. García, Tip motion in amplitude modulation (tapping-mode) atomic-force microscopy: Comparison between continuous and point-mass models, *Appl. Phys. Lett.*, **80**, 1646–1648 (2002).