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INFLUENCE OF THE PROBE SPRING CONSTANT AND THE QUALITY FACTOR ON ITS OSCILLATION CHARACTERISTICS IN DYNAMIC MODE OF ATOMIC FORCE MICROSCOPY

Abstract. The work presents the results of mathematical simulation of dynamic atomic force microscopy (AFM). Influences of spring constant, the quality factor of AFM-probe on its vibration amplitude and phase shifts are studied for semi-contact interaction of tip probe and sample surface. The deformation depths of sample by probe are calculated. Also the influence of oscillation amplitude of piezogenerator, which forces probe vibration, on the characteristics of probe oscillation is shown.

Keywords: atomic force microscopy, AFM, dynamic mode, probe, oscillation, the Johnson–Kendall–Roberts model, probe spring constant, the probe quality factor, oscillation amplitude of piezogenerator, deformation depth of material

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ВЛИЯНИЕ ЖЕСТКОСТИ И ДОБРОТНОСТИ ЗОНДА НА ХАРАКТЕРИСТИКИ ЕГО КОЛЕБАНИЙ В ДИНАМИЧЕСКОМ РЕЖИМЕ РАБОТЫ АТОМНО-СИЛОВОГО МИКРОСКОПА

Аннотация. В работе приведены результаты математического моделирования динамической атомно-силовой микроскопии (АСМ). Исследовано влияние жесткости и добротности АСМ-зонда на амплитуду, сдвиг фазы колебаний его острия в режиме полуконтактного взаимодействия с поверхностью материала. Рассчитаны глубины деформирования материала зондом. Также показано влияние амплитуды колебаний пьезогенератора, вынуждающего зонд осциллировать, на характеристики колебаний зонда.

Ключевые слова: атомно-силовая микроскопия, АСМ, динамический режим, зонд, колебания, модель Джонсона–Кенделла–Робертса, жесткость зонда, добротность зонда, амплитуда колебаний пьезогенератора, глубина деформирования материала

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Introduction. Dynamic atomic force microscopy (AFM) remains one of the most popular methods for studying material surfaces. Despite the appearance of such specific modes as Force modulation mode, Peak Force Tapping™, Lift mode operation, Pulsed Force Mode, ScanAsyst®, high-speed AFM, the classic tapping mode is one of the leading ones. Its capabilities are wider in comparison with the most popular contact AFM, but its setup is also much more complicated. The complexity is enhanced by the fact that parameters for obtaining AFM images, which are "ideal" for one sample material, may be unsuitable for another sample with similar physical and mechanical characteristics.

The most common measurement errors on AFM images are defects like "break" type, which appear as noise on images and do not represent the actual relief of sample surface. Such noises are located on image in the direction of scanning the sample. They can be a consequence of incorrect adjustment of the

AFM feedback parameters or arise due to relatively high adhesion of surface of the scanned sample. The noises associated with the latter could be avoided by changing the characteristics of the dynamic interaction of probe with sample due to the selection of probe parameters.

The characteristics of probe-sample interaction (amplitude and phase shift of probe oscillations, deformation depth of sample by probe) are influenced by a set of parameters: the Young modulus and surface energy of sample; the spring constant and the quality factor of probe; oscillation amplitude of the piezoelectric generator (piezoelectric element) exciting probe oscillations.

The average spring constant of probe cantilever is specified by probe manufacturer; the probe quality factor is not given. Sometimes probes with calibrated stiffness are offered. The AFM operators could determine the spring constant and the quality factor of probe independently using its amplitude-frequency characteristic with AFM dynamic mode. The range of probe spring constant offered by manufacturers for tapping mode is wide, from 0.03 to 225 N/m [1–6].

For selection the characteristics of probe and oscillation amplitude of piezoelectric generator to avoid noises on AFM images, it is necessary to find out at what changes of these parameters switching of the probe-sample interaction modes occurs. In [7] reported that during AFM scanning of samples in tapping mode spontaneous switching between modes of higher or lower probe oscillation amplitude can occur, and causing defects of "break" type in AFM images. It was previously shown that saltatory changes in curves of dependence of probe oscillation amplitude and phase shift on the distance between probe and sample are caused by an interchange in the predominance of attractive intermolecular or repulsive (elastic) interaction forces between probe and sample [8].

The purpose and objectives of the study. The objective of the study is to identify the pattern of changes in the probe oscillation parameters under varying each of the probe characteristics separately (the spring constant, the quality factor) and piezogenerator oscillation amplitude in order to obtain recommendations for select probes for high-quality AFM images in the tapping mode of AFM.

Research method. The equation of probe oscillations during semi-contact (intermittent-contact) interaction with sample was solved using mathematical simulation methods. The model (1), developed earlier and corresponding well to the experimental data, was used [9]. At this model non-contact attractive interactions for describing the process of approaching probe tip to sample during each cycle of probe oscillations are taken into account using the Lennard–Jones potential. The contact interaction of probe and sample, occurring in the lower part of a probe oscillation cycle, is described according to the Johnson–Kendall–Roberts model for elastic-adhesive contact of a sphere and a plane [10].

The equation of probe oscillations is

$$mz'' + \frac{m\omega_0}{Q} z' + k(z - z_{\text{pos}}) = a_{\text{bm}} k \sin(\omega t) + F_{\text{ts}}(z), \tag{1}$$

where the force of interaction between probe and sample surface is

$$F_{\text{ts}}(z) = \begin{cases} F_{\text{LJ}}(z), & z > z_{F0} \\ F_{\text{JKR}}(z), & z \le z_{F0} \end{cases}, \quad F_{\text{LJ}}(z) = -\frac{HR}{6}\left(\frac{1}{z^2} - \frac{\sigma^6}{4z^8}\right), \quad F_{\text{JKR}}\left(\frac{z}{z_c}\right) = \left(\frac{z}{z_c}\left(\frac{F_{\text{JKR}}}{P_c}\right)\right)^{-1},$$

$$\frac{z}{z_{\text{c}}} = \begin{cases} -\left(3\sqrt{\dfrac{F_{\text{JKR}}}{P_c}+1}-1\right)\left[\dfrac{1}{9}\left(\sqrt{\dfrac{F_{\text{JKR}}}{P_c}+1}+1\right)\right]^{1/3}, & \dfrac{z}{z_c} \le 3^{-2/3}, \\ \left(3\sqrt{\dfrac{F_{\text{JKR}}}{P_c}+1}+1\right)\left[\dfrac{1}{9}\left(1-\sqrt{\dfrac{F_{\text{JKR}}}{P_c}+1}\right)\right]^{1/3}, & 3^{-2/3} \le \dfrac{z}{z_c} \le 1, \end{cases} \quad z_c = \frac{1}{3R}\left(\frac{3RP_c}{k_s}\right)^{2/3}, \quad P_c = \frac{3}{2}\pi R \Delta\gamma,$$

$$\Delta\gamma = \frac{H}{16\pi\sigma^2}, \quad k_s = \frac{4}{3\pi}\frac{1}{\kappa_1 + \kappa_2}; \quad \kappa_i = \frac{1-\nu_i^2}{\pi E_i}, \quad i = \overline{1, 2}.$$

Initial conditions are $z(0) = z_{\text{pos}}$, $z'(0) = 0$.

Here z_{pos} is a position of cantilever fixing point above sample surface, nm; m is a mass of microprobe, kg; z is a vertical displacement of tip probe, nm; t is a time, s; ω_0 is a natural angular frequency of probe, Hz; Q is the quality factor of cantilever; k is the spring constant of probe cantilever, N/m; a_{bm} is oscillation amplitude of piezoelement, on which cantilever is fixed, nm; ω is an operating angular frequency of probe, Hz; F_{ts} is an interaction force between probe and sample surface, nN; F_{LJ} is a non-contact interaction force, nN; F_{JKR} is a contact interaction force according to the Johnson–Kendall–Roberts model, nN; z_{F0} is a distance, at which contact and non-contact interaction forces are balanced, nm; H is the Hamaker constant, aJ; R is a radius of probe tip curvature, nm; σ is an interatomic distance, nm; P_c is the maximum force of adhesion, nN; $\Delta\gamma$ is a specific surface energy of sample, J/m^2; k_s is the reduced modulus of elasticity of sample and tip materials, GPa; ν_1, ν_2 are the Poisson's ratios of tip and sample materials, respectively; E_1, E_2 are the Young moduli of tip sample materials, respectively, GPa; aJ = 10^{-18} J – attojoule.

Since the distance z_{pos} between probe cantilever fixing point and sample is changed during AFM scanning of sample surface, the simulation was performed for z_{pos} from zero to values close to values of free oscillation amplitude of probe A_0. A height of probe tip was neglected.

Based on the simulation results, the graphs were constructed for dependences of amplitude, phase shift of probe oscillations, and for deformation depth of sample material on the distance between probe and sample.

In order to study influence of probe parameters and piezogenerator oscillation amplitude, the characteristics of sample were assumed to be constant: the Young modulus was equal to 0.1 GPa; the Hamaker constant, responsible for surface energy, was equal to 0.2 aJ. Then, two of the studied parameters were fixed in turn and the third was varied. When varying spring constant of probe cantilever (from 0.01 to 100 N/m), its quality factor Q was assumed to be equal to 100, the oscillation amplitude of piezoelement a_{bm} = 0.5 nm. During changing the quality factor of the probe (from 80 to 400), its spring constant k = 0.5 N/m, a_{bm} = 0.5 nm. When studying influence of piezoelement oscillation amplitude (from 0.1 to 2 nm), k = 0.5 N/m, Q = 100. The radius of probe tip curvature was taken to be equal to 10 nm. The Young modulus of probe tip was equal to 179 GPa and corresponds to silicon. Deformation depth of sample surface by probe tip was $d = z - z_{F0}$ [nm]. For each curve, 40 points were calculated.

Results and discussion. Cantilevers with the spring constant of 5–100 N/m are suitable for scanning a sample with the specified characteristics, since the corresponding curves of probe oscillation amplitude do not have abrupt changes (Fig. 1, *a*), and the phase shift curves are located in the region of negative values (Fig. 1, *b*), which indicates the predominance of the elastic mode of interaction between probe and sample [8] and is confirmed by the positive values of the probe-sample interaction force (Fig. 1, *d*). A disadvantage of the probe spring constant of 20–100 N/m is rather high values of the sample deformation depth (Fig. 1, *c*). At such values of the cantilever spring constant, its oscillations do not damp at zero distance to sample surface. The probe continues to oscillate, penetrating into sample surface by 15–32 nm. The greater sample deformation depth during scanning causes the higher errors in height of sample relief on AFM images. In this sense, the probe spring constant of 5 N/m can be called "ideal" (for samples with a sufficiently developed relief), since the maximum sample deformation depth does not exceed 8 nm.

At k = 0.5 N/m, a jump-like switching between the mode of prevalence of probe-sample elastic repulsive forces and the mode of prevalence of attractive interaction between them is observed (Fig. 1). The mode of prevalence of elastic forces corresponds to a higher located branch of the probe oscillation amplitude, a negative phase shift, positive values of the sample deformation depth and the probe-sample interaction force at the bottom point of the probe oscillation cycle. Accordingly, attractive interactions are indicated by a lower branch of the probe oscillation amplitude, a positive phase shift, a negative (although small in values) interaction force and zero sample deformation depth. Scanning sample in the regime of prevalence of attractive interactions actually means the implementation of the non-contact AFM mode.

A further decrease of the probe spring constant (k = 0.1 N/m) shows that the non-contact attractive mode is realized for this sample for almost all values of the distance z_{pos}. At z_{pos} < 10 nm, the probe stops

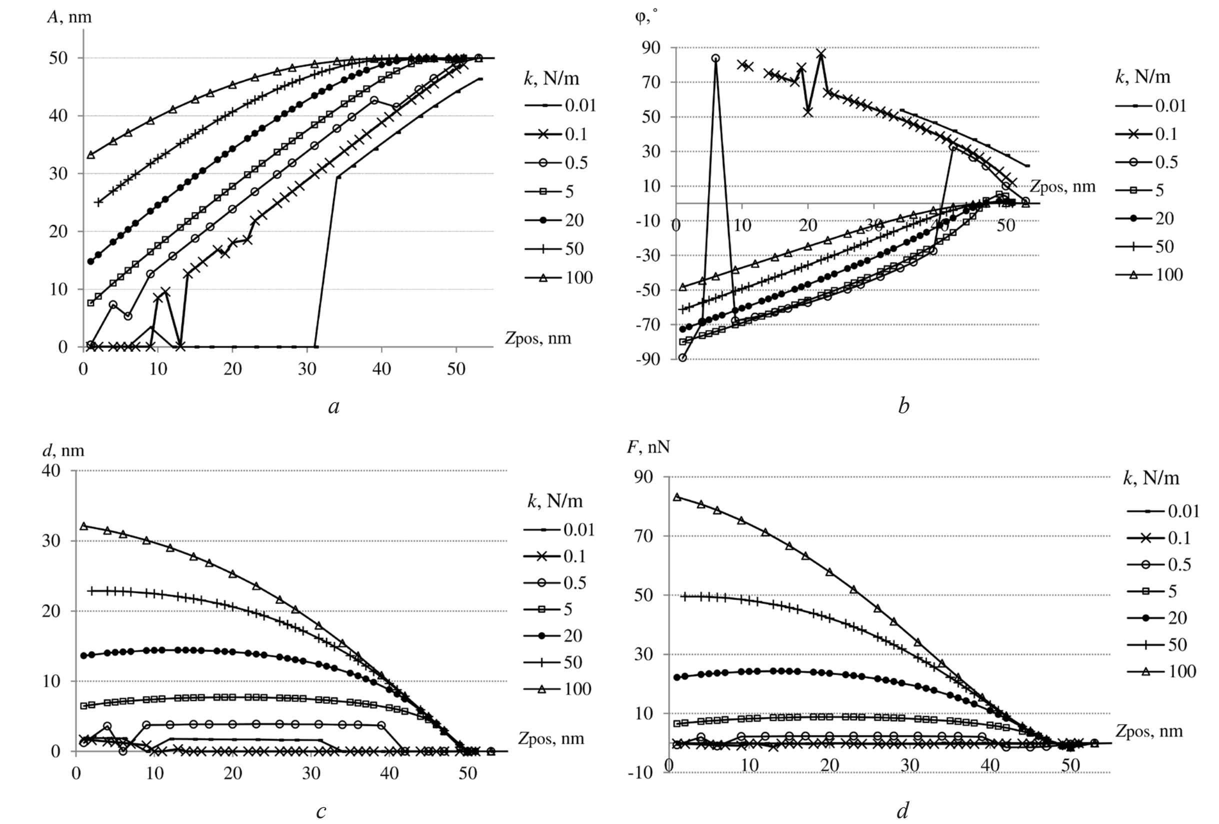

Fig. 1. Dependences of the oscillation characteristics of probes with different spring constants on distance between probe and sample: amplitude A (*a*); phase shift φ (*b*); sample deformation depth (*c*); interaction force F of probe and sample at the bottom point of a probe oscillation cycle (*d*). Q = 100, a_{bm} = 0.5 nm

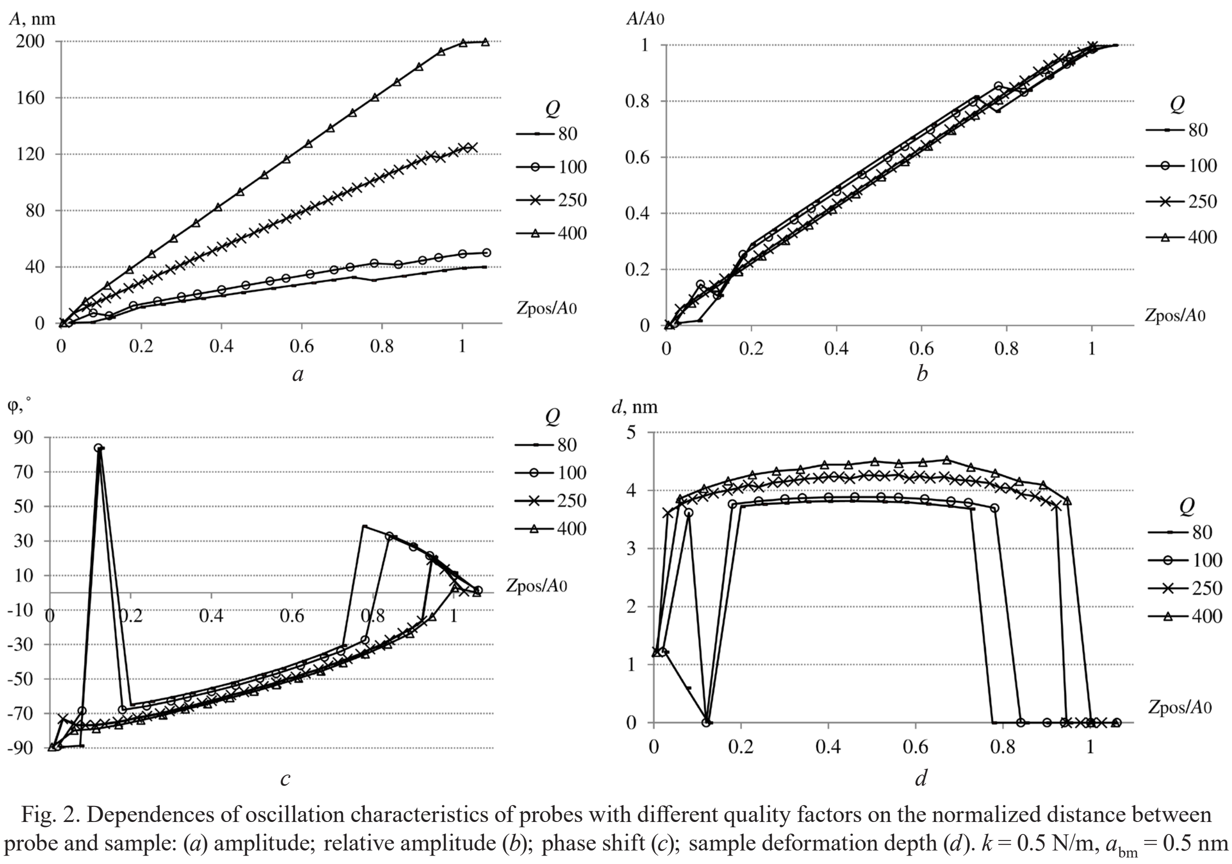

Fig. 2. Dependences of oscillation characteristics of probes with different quality factors on the normalized distance between probe and sample: (*a*) amplitude; relative amplitude (*b*); phase shift (*c*); sample deformation depth (*d*). k = 0.5 N/m, a_{bm} = 0.5 nm

oscillating (Fig. 1, *a*), and the sample deformation depth becomes, although small, non-zero (d = 1.5 nm). This indicates that probe adheres to sample surface, i. e., the surface adhesion of sample becomes critically significant at the probe spring constant of 0.1 N/m.

At k = 0.01 N/m, the sample adhesion effect increases, the probe adheres to it already at z_{pos} = 32 nm, and the probe tip remains immersed in the sample by 2 nm.

Varying the probe quality factor shows similar results with respect to switching the interaction modes of the probe and sample: switching from the mode of predominance of elastic forces to the mode of attraction predominance is realized faster, when the probe quality factor is lower (Fig. 2). However, unlike the probe spring constant, its quality factor has an insignificant effect on the sample deformation depth: less than 1 nm for this sample under changing of Q in a fairly wide range, from 80 to 400 (Fig. 2, *d*). Therefore, to achieve the best scanning results, higher values of the probe quality factor are preferable.

The probe behavior under varying the oscillation amplitude of the piezogenerator is generally similar to the behavior when the probe spring constant is changed: when the a_{bm} values decrease, abrupt switches from the mode of predominance of elastic forces to the mode of predominance of attractive interactions of the probe and the sample are observed; a decrease in the a_{bm} values to 0.3 nm and below leads to the non-contact mode of probe oscillations, which are damped at a small distance to the sample (Fig. 3). The sample deformation depth increases with increase of the oscillations amplitude of the piezogenerator, but not as significantly as with increase of the probe spring constant (Fig. 1, *c* and 3, *d*).

To obtain high-quality AFM images of the sample with the Young modulus of 0.1 GPa and the Hamaker constant of 0.2 aJ, the following parameter combinations are "ideal": k = 5 N/m, Q = 100, a_{bm} = 0.5 nm (Fig. 1); Q = 400, k = 0.5 N/m, a_{bm} = 0.5 nm (Fig. 2), a_{bm} = 2 nm, k = 0.5 N/m, Q = 100 (Fig. 3). For material samples with other characteristics, modes suitable for scanning may occur under other conditions.

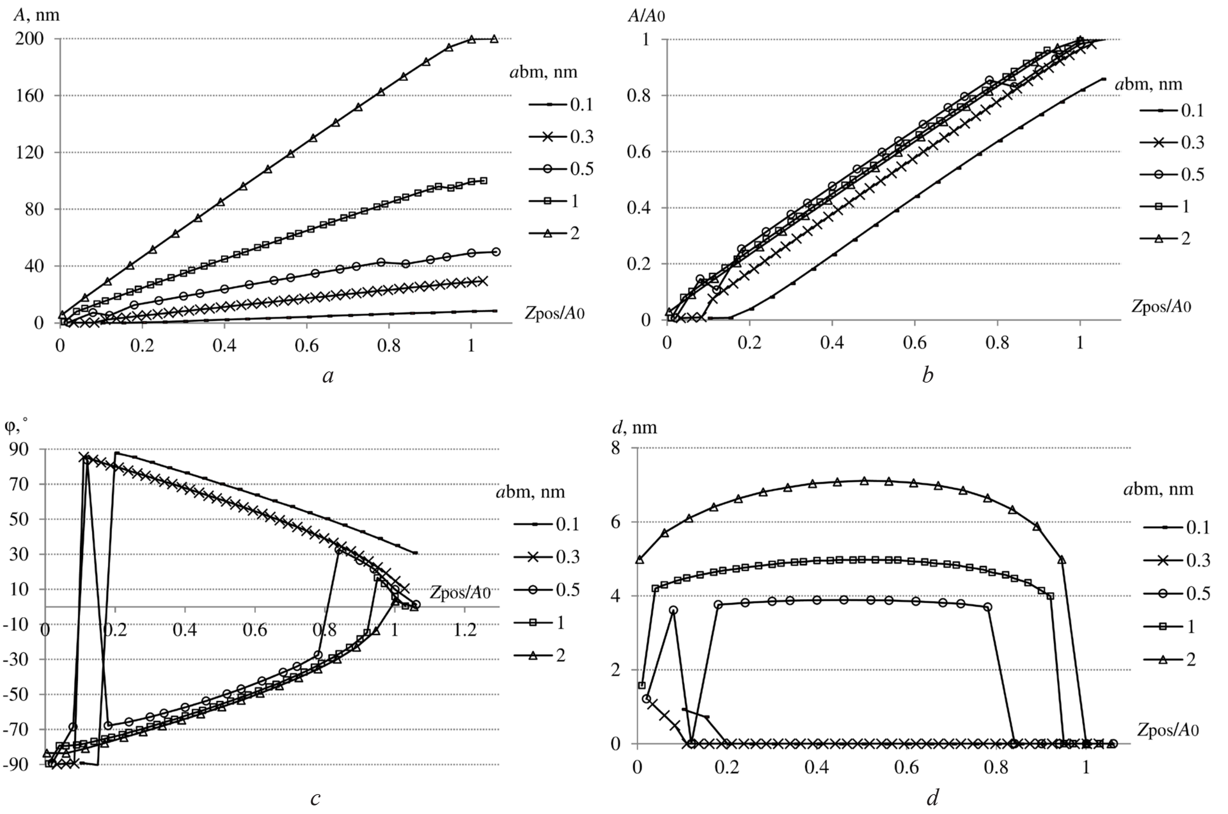

Fig. 3. Dependences of oscillation characteristics of probe on the normalized distance between probe and sample under varying oscillation amplitude of piezoelement: amplitude of probe oscillations (*a*); relative amplitude of probe oscillations (*b*); phase shift (*c*); sample deformation depth (*d*). k = 0.5 N/m, Q = 100

Conclusion. The efficiency of the model for defining the conditions for switching between the modes of predominantly attractive or repulsive interactions between probe and sample is demonstrated using one material as an example. It was found that the following parameter combinations are "ideal" in order to obtain high-quality AFM images of the sample with the Young modulus of 0.1 GPa and the Hamaker constant of 0.2 aJ. For the quality factor Q = 100 and the piezoegenerator oscillation amplitude a_{bm} = 0.5 nm, the most suitable probe spring constant is k = 5 N/m; decreasing the spring constant to values of 0.5 or less leads to abrupt changes in the probe oscillation characteristics. For the probe spring constant k = = 0.5 N/m, a_{bm} = 0.5 nm, the best quality factor is Q = 400, and decreasing the quality factor to 250 or less leads to switching between the modes of attraction and repulsion of probe and sample. For the probe with characteristics k = 0.5 N/m, Q = 100, the "ideal" amplitude is a_{bm} = 2 nm; its reduction to 1 nm or less shows abrupt changes in the curves.

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