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Evaluation of the capacitive force between an atomic force microscopy tip and a metallic surface

S. Hudlet, M. Saint Jean[a], C. Guthmann, and J. Berger

Groupe de Physique des Solides, Universités Paris 6 et 7, Tour 23, 2 place Jussieu, 75251 Paris Cedex 05, France

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Abstract. We propose a very simple method to determine the electrical tip-surface force in Atomic Force Microscopes used to study the electrical properties of metallic or insulating materials; the analysis of the measurements as well as determination of the appropriate experimental procedures requiring an analytical model of the tip-surface capacitance. The comparison of force expressions obtained by this method with those obtained by exact derivation in the case of the sphere-infinite plane system shows very good agreement. This method is then applied to determine the tip-surface force, the real shape of the tip being introduced in the derivation. The obtained expression is compared to experimental and numerical data. We emphasize that this method is very general and can be applied to any axially symmetric capacitor.

PACS. 06.30.-k Measurements common to several branches of physics and astronomy – 07.50.-e Electrical and electronic components, instruments, and techniques – 41.20.-q Electric, magnetic, and electromagnetic fields

Scanning microscopies have recently been used to study the electrical properties of metallic or insulating materials, eventually coated by absorbed films. In all these techniques, a metallic tip scans a thin sample fixed on a conducting surface. When a potential is applied between the tip and the underlying metallic surface, such a system forms an axially symmetric capacitor. The tip is then submitted to an electric force, proportional to the capacitance gradient. Since this capacitance depends on surface properties and the tip-surface distance (the cantilever-surface contribution may be neglected), we can obtain topographic and local electrical properties of the surface by measuring the tip-surface force. However, interpretation of these measurements as well as determination of the appropriate experimental procedures require an analytical model of the tip-surface capacitance.

Various methods have been developed to calculate the capacitance of conductors at equilibrium. Unfortunately, these methods are not always analytical, even for highly symmetric systems, and numerical methods are used. Applied to the AFM tip-metallic surface case, these numerical methods give the exact determination of the force, but they do not offer the opportunity to directly discuss the influence of the relevant experimental parameters (tip dimension, apex radius, tip- surface distance...) on the obtained measurements. To remove these difficulties, we have developed an original analytical derivation of the electric field created by a convex metallic system with axial symmetry, applied to the tip-surface system. This method allows an approximate analytical determination of the tip-surface capacity and of the tip-surface force.

[a] e-mail: saintjean@gps-jussieu.fr

1 Description of the method and its validation

Let us consider an axial capacitor constituted by an infinite plane surface and an axial symmetric electrode (hereafter called the tip) which are respectively maintained at the potentials $V = 0$ and V (Fig. 1). The vertical force applied on the tip is given by:

$$F_z = \int_{\mathrm{s}} \frac{\sigma^2}{2\varepsilon_0} \mathrm{d}S\ \mathbf{n} \cdot \mathbf{u}_z \tag{1}$$

where σ is the aeral charge density on the infinitesimal surface $\mathrm{d}S$ of the tip, $\mathbf{n}$ being the unitary vector normal to this surface. The local charge density σ is related to the electric field on the metallic tip surface by:

$$E = \frac{\sigma}{\varepsilon_0} \cdot$$

Then, to evaluate the tip-surface force F_z, it is necessary to determine the electric field at each point on the tip. This determination requires the resolution of the Laplace equation taking into account the conditions imposing a constant voltage on the metallic surfaces. An analytical solution is not always possible, so we have developed an analytical method which gives an approximate expression of this field.

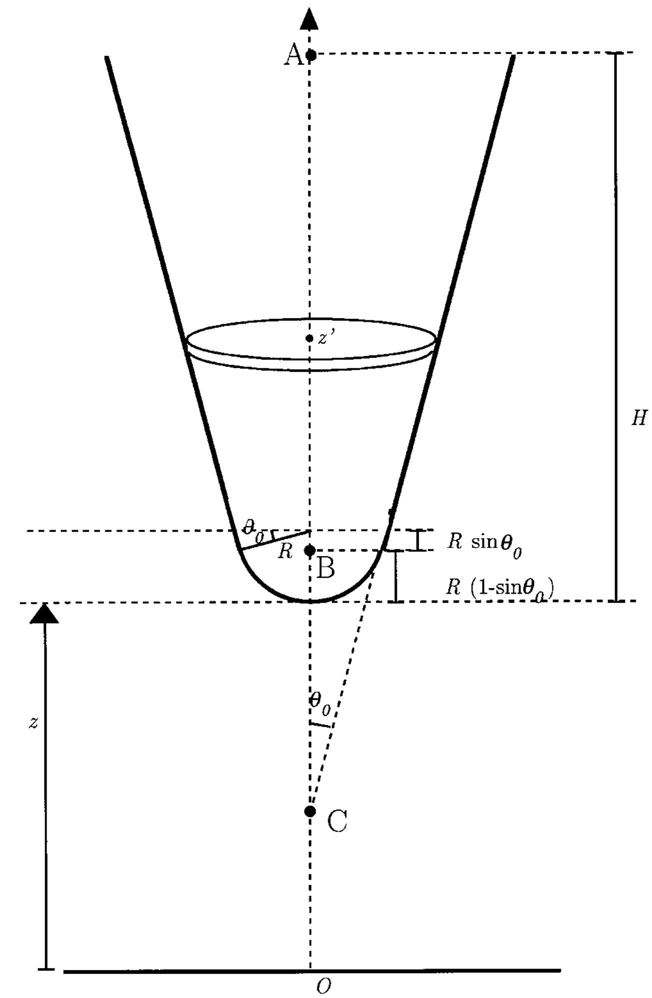

Fig. 1. Tip-infinite flat surface system and characteristic dimensions.

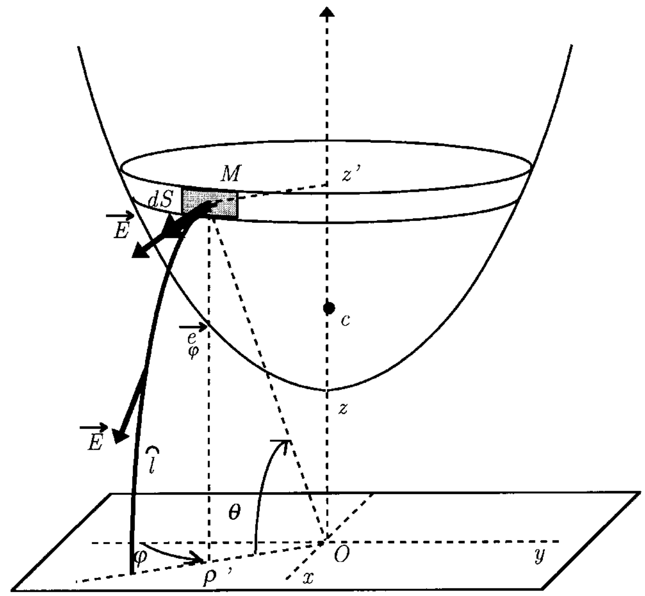

Fig. 2. Facetted tip-infinite flat surface and approximate field lines.

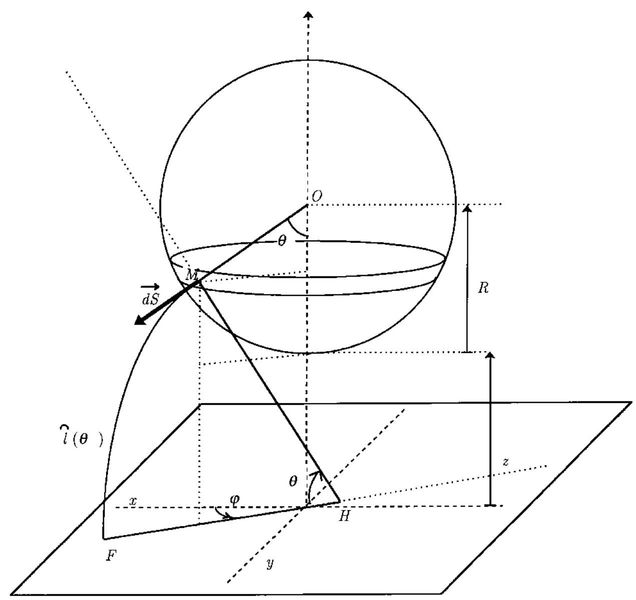

Fig. 3. Sphere-infinite flat surface.

In our method, the first step is to identify the tip surface as a superposition of infinitesimal surfaces obtained by facetting (Fig. 2). Thus, from an electrostatic point of view, for distances greater than the characteristic facet dimensions, the tip surface appears as regular; since the roughness is infinitesimal we can hope to obtain the right expression whatever the tip surface distance. The second step is to evaluate the electric field created between this facetted conductor and the plane surface. To obtain this field, we postulate that the electric field on each infinitesimal tip surface is that which would be created by the dihedral capacitance constituted by two infinite planes in the same relative orientation. This is the main approximation of our model. This approximate field is introduced in expression (1) to determine the infinitesimal force $\mathrm{d}F_z$ and the tip-surface force can be finally obtained by summing all these contributions.

To illustrate this method and test its validity, we first calculate the force between a sphere and an infinite plane since this geometry allows a comparison between our derivation and the exact one. Then we will consider the sphere presented in Figure 3, its radius and its distance to the planar surface being respectively denoted R and z. On each point $M(R,\theta,\varphi)$ of this sphere we can construct an infinitesimal surface $\mathrm{d}S = R^2 \sin\theta \mathrm{d}\theta \mathrm{d}\varphi$. We assume that the electric field on this point is then equal to:

$$E = -\frac{V}{l(M)}$$

where $l(M)$ is the length of the field line of the corresponding dihedral capacitor

$$l(M) = \frac{\theta[z + R(1-\cos\theta)]}{\sin\theta}\,.$$

Knowing the electric field we can deduce the charge density:

$$\sigma(M) = -\frac{\varepsilon_0 V \sin\theta}{\theta[z + R(1-\cos\theta)]}\,.$$

The sphere-surface force can then be derived using relation (1). However, since the sphere and the infinite plane are in total influence, it is more convenient to calculate the sphere-plane capacitance to determine this force. This capacitance is given by the following expression:

$$C(z) = 2\pi\varepsilon_0 R \int_0^{\pi} \frac{\sin^2\theta}{\theta\left[\frac{z}{R} + 1 - \cos\theta\right]}\mathrm{d}\theta.$$

The integral part $I(z, R)$ of this capacitance cannot be analytically evaluated. However, we can estimate its variation with distance z by surrounding this integral by two other integrals having the same distance dependence:

$$\int_0^{\pi/2} \frac{\sin^2\theta}{\theta\left[\frac{z}{R} + 1 - \cos\theta\right]}\mathrm{d}\theta < \int_0^{\pi} \frac{\sin^2\theta}{\theta\left[\frac{z}{R} + 1 - \cos\theta\right]}\mathrm{d}\theta < 2\int_0^{\pi/2} \frac{\sin^2\theta}{\theta\left[\frac{z}{R} + 1 - \cos\theta\right]}\mathrm{d}\theta.$$

This inequality is justified by the fact that the charge on the sphere is principally located on the hemisphere near the planar surface. Moreover, we have:

$$\int_0^{\pi/2} \frac{\sin^2\theta}{\theta\left[\frac{z}{R} + 1 - \cos\theta\right]}\mathrm{d}\theta < \int_0^{\pi/2} \frac{\sin^2\theta}{\left[\frac{z}{R} + 1 - \cos\theta\right]}\mathrm{d}\theta = \ln(1 + \frac{R}{z})$$

since $\theta > \sin\theta$ over the interval $(0,\ \pi/2)$ and

$$\int_0^{\pi/2} \frac{\sin^2\theta}{\theta\left[\frac{z}{R} + 1 - \cos\theta\right]}\mathrm{d}\theta > \frac{4}{\pi^2}\int_0^{\pi/2} \frac{\theta}{\left[\frac{z}{R} + \frac{\theta^2}{2}\right]}\mathrm{d}\theta = \frac{4}{\pi^2}\ln(1 + \frac{\pi^2}{8}\frac{R}{z}) > \frac{4}{\pi^2}\ln(1 + \frac{R}{z})$$

since $1 - \cos\theta < \theta^2/2$ and $\sin\theta > 2\theta/\pi$ ($\sin\theta$ is convex over the interval $(0,\ \pi/2)$). Then, whatever the tip-surface distance, we can write:

$$\frac{4}{\pi^2}\ln(1 + \frac{R}{z}) < \int_0^{\pi} \frac{\sin^2\theta}{\theta\left[\frac{z}{R} + 1 - \cos\theta\right]}\mathrm{d}\theta < 2\ln(1 + \frac{R}{z}).$$

Following this inequality, we can assume that the integral $I(z,\ R)$ can be written:

$$I = K\ln(1 + \frac{R}{z})$$

where K is a constant which has to be determined. By introducing this relation in the expression of the sphere-surface force given by:

$$F_z(z) = -\frac{\partial C}{\partial z}\frac{V^2}{2}$$

we obtain:

$$F_z(z) = 2\pi\varepsilon_0 K \left[\frac{R^2}{z(z+R)}\right]\frac{V^2}{2}\,. \tag{2}$$

To determine the constant K, we have compared the exact and approximate solutions in the asymptotic limit $z \gg R$. The exact expression of the force between the sphere and the plane calculated by the image method [2] is given by:

$$F_z(z) = V^2 2\pi\varepsilon_0 \sum_{n=1}^{\infty} \frac{\coth\,\alpha - n\coth\,n\alpha}{\mathrm{sh}\,n\alpha}$$
$$\mathrm{ch}\,\alpha = 1 + z/R. \tag{3}$$

When the sphere is very far from the surface, this last expression can be simplified and we obtain:

$$F_z = \pi\varepsilon_0\left(\frac{R}{z}\right)^2 V^2. \tag{4}$$

The comparison of expressions (2) and (4) gives $K = 1$. Thus the final expression of the sphere-plane force is given in our method by:

$$F_z(z) = \pi\varepsilon_0\left[\frac{R^2}{z(z+R)}\right]V^2. \tag{5}$$

The variations of force given by expressions (3, 5) *versus* the sphere-surface distance are presented in Figures 4a and 4b respectively for ($0 < z < 100$ nm) and higher distances, using $R = 20$ nm. Whatever the distance, very good agreement between the two derivations can be observed. More quantitatively, the error is less than 1% for small ($z/R < 0.01$) and large ($z/R > 4$) distances, with the maximum error (5%) being found for z about $R/3$. So, we have used it to derive the tip-surface force in an Atomic Force microscope.

2 Capacitive force associated with an axially symmetric metallic capacitor

The tip shape and its characteristic dimensions are determined by electronic microscopy. It can be modelled as a truncated cone ended by a spherical apex. Figure 1 introduces all the geometric characteristic of this tip. We shall now evaluate separately the apex and conic contributions.

2.1 Spherical contribution

The spherical apex is characterized by the radius of curvature R and its angular aperture $2\theta_0$. Extending the procedure proposed in the previous section, the electric charge

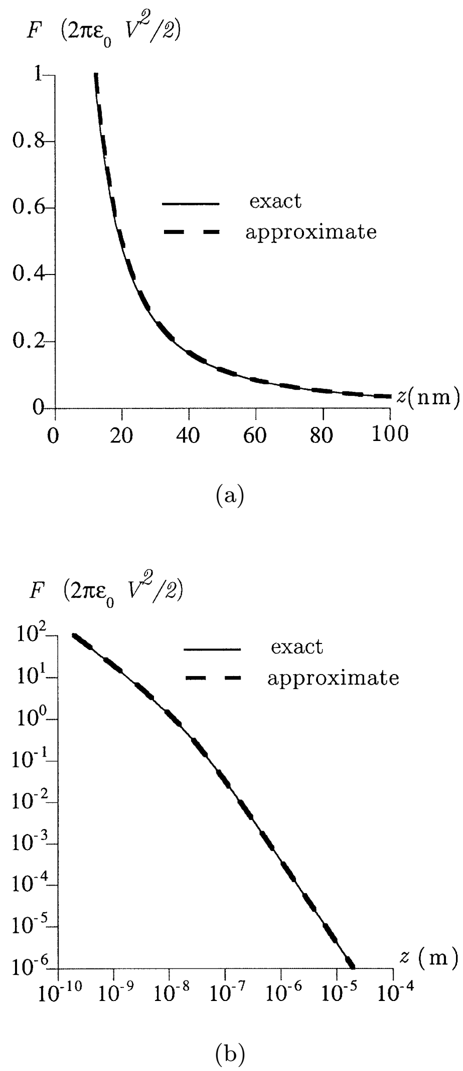

Fig. 4. (a) Comparison between exact and approximate forces for ($0 < z < 100$ nm) and $R = 20$ nm; (b) Comparison between exact and approximate forces for (10^{-10} m $< z < 10^{-4}$ m) and $R = 20$ nm.

accumulated on this apex can be calculated and its expression is

$$\delta Q(z) = 2\pi\varepsilon_0 RV \int_0^{\pi/2-\theta_0} \frac{\sin^2\theta}{\theta\left[\frac{z}{R}+1-\cos\theta\right]}\mathrm{d}\theta$$
$$\delta Q(z) = 2\pi\varepsilon_0 RV I_{\theta_0}(z/R).$$

The usual values of θ_0 are around 10°, so we can consider that:

$$\frac{\sin(\pi/2-\theta_0)}{\pi/2-\theta_0} < \frac{\sin\theta}{\theta} < 1.$$

Then we can write:

$$\frac{\cos\theta_0}{\pi/2-\theta_0}\int_0^{\pi/2-\theta_0} \frac{\sin\theta}{\left[\frac{z}{R}+1-\cos\theta\right]}\mathrm{d}\theta < I_{\theta_0}(z/R) < \int_0^{\pi/2-\theta_0} \frac{\sin\theta}{\left[\frac{z}{R}+1-\cos\theta\right]}\mathrm{d}\theta \cdot$$

and

$$\frac{\cos\theta_0}{\pi/2-\theta_0}\ln\frac{z+R(1-\sin\theta_0)}{z} < I_{\theta_0}(z/R) < \ln\frac{z+R(1-\sin\theta_0)}{z}.$$

This inequality suggests describing the apex contribution by a capacitance given by:

$$C_{\mathrm{apex}} = 2\pi\varepsilon_0 RK' \ln\frac{z+R(1-\sin\theta_0)}{z}$$

the corresponding contribution to the tip-surface force is equal to:

$$F_{\mathrm{apex}} = \pi\varepsilon_0 RK' \frac{R(1-\sin\theta_0)}{z[z+R(1-\sin\theta_0)]}V^2 \cdot \qquad (6)$$

To determine K' we consider the situation where the tip is very close to the surface. In this case, the apex contribution is dominant and can be identified with the force exerted by the plane on a complete sphere in the same conditions ($z \ll R$). By comparing expressions (3) and (6), we obtain $K' = 1$. Thus the apex contribution can be written:

$$F_{\mathrm{apex}} = \pi\varepsilon_0 R^2 \frac{(1-\sin\theta_0)}{z[z+R(1-\sin\theta_0)]}V^2 \cdot$$

2.2 Conical contribution

We now have to calculate the conical contribution. At a height z', each point on the conical part of the tip is associated with $l(M)$ given by:

$$l(M) = (\frac{\pi}{2}-\theta_0)MH = (\frac{\pi}{2}-\theta_0)\frac{z'}{\cos\theta_0}$$

the charge density at this point is then:

$$\sigma(M) = \frac{-\varepsilon_0 V\cos\theta_0}{(\frac{\pi}{2}-\theta_0)z'}$$

and the force contribution:

$$F_{\mathrm{cone}} = \frac{\pi\varepsilon_0 V^2\sin^2\theta_0}{(\pi/2-\theta_0)^2}\int_{z_{\mathrm{B}}}^{z_{\mathrm{A}}} \frac{(z'-z_{\mathrm{C}})}{z'^2}\mathrm{d}z'$$

$$F_{\mathrm{cone}} = \frac{\pi\varepsilon_0 V^2\sin^2\theta_0}{(\pi/2-\theta_0)^2}\left[\ln\frac{z_{\mathrm{A}}}{z_{\mathrm{B}}} + z_{\mathrm{C}}\left(\frac{1}{z_{\mathrm{A}}}-\frac{1}{z_{\mathrm{B}}}\right)\right].$$

If we consider the particular case $z_{\mathrm{C}} = 0$ and $z_{\mathrm{B}} = \delta \ll z_{\mathrm{A}}$ the cone contribution can be reduced to :

$$F_{\mathrm{cone}} = \frac{\pi\varepsilon_0 V^2 \sin^2\theta_0}{(\pi/2-\theta_0)^2}\ln\frac{H}{\delta}\,. \tag{7}$$

For this particular geometry where $H \gg \delta$, the usual assumption is to consider the field lines as identical to those obtained for an infinite cone. In this frame, the "exact" expression of the force can be identified with the force contribution which applies on the part H of an infinite cone [3,4]. This force is equal to:

$$F_{\mathrm{cone}} = \frac{\pi\varepsilon_0 V^2}{[\ln\,\mathrm{tg}(\theta_0/2)]^2}\ln\frac{H}{\delta}\,. \tag{8}$$

As for the sphere-plane example, the variations of force with tip-surface distance are similar in the exact and approximate expressions. As done above, to make precise the approximate force expression, we identify the prefactor obtained in the approximate expression with its value in the exact derivation of the particular case. (Notice that the prefactors present similarity for large angle θ_0.) Then the conic contribution is given by:

$$F_{\mathrm{cone}} = \frac{\pi\varepsilon_0 V^2}{[\ln\,\mathrm{tg}(\theta_0/2)]^2}\left[\ln\frac{z_{\mathrm{A}}}{z_{\mathrm{B}}} + z_{\mathrm{C}}\left(\frac{1}{z_{\mathrm{A}}}-\frac{1}{z_{\mathrm{B}}}\right)\right]. \tag{9}$$

In the tip geometry, $z_{\mathrm{A}} \gg z_{\mathrm{B}}$ and z_{C}, then $\ln(z_{\mathrm{A}}/z_{\mathrm{B}}) \approx -\ln(z_{\mathrm{B}}/H)$ and $z_{\mathrm{C}}/z_{\mathrm{A}}$ is neglected. So, after introducing the continuity condition between the apex and the cone, we obtain finally:

$$F_{\mathrm{total}} = \pi\varepsilon_0 V^2\left[\frac{R^2(1-\sin\theta_0)}{z[z+R(1-\sin\theta_0)]} + k^2\left(\ln\frac{z+R(1-\sin\theta_0)}{H} - 1 + \frac{R\cos^2\theta_0/\sin\theta_0}{z+R(1-\sin\theta_0)}\right)\right]$$

where

$$k^2 = \frac{1}{[\ln\mathrm{tg}(\theta_0/2)]^2}\,.$$

For the tip used in our microscope, θ_0 is small. In this case, this last force expression can be simplified and we obtain:

$$F_{\mathrm{total}} = \pi\varepsilon_0 V^2\left[\frac{R^2}{z[z+R]} + k^2\left(\ln\frac{z+R}{H} - 1 + \frac{R/\sin\theta_0}{z+R}\right)\right].$$

This expression can be examined for different asymptotic limits. When the tip is very close to the surface, $z \ll R$, the tip-surface force varies as $\pi\varepsilon_0 R/z$, whereas it varies as $\pi\varepsilon_0 k^2\ln(H/z)$ for $z \gg R$. This means that the force, and thus the images, are controlled by the apex radius near the surface and by the tip dimensions as soon as the tip surface distance is larger than R. Notice that these asymptotic results correspond to the different models previously presented in the literature for a restricted tip-surface distance range, and can be used for these particular limits [4,5]. For intermediate tip-surface distances such as those used in AFMR, the complete expression must be employed in discussing the experimental data.

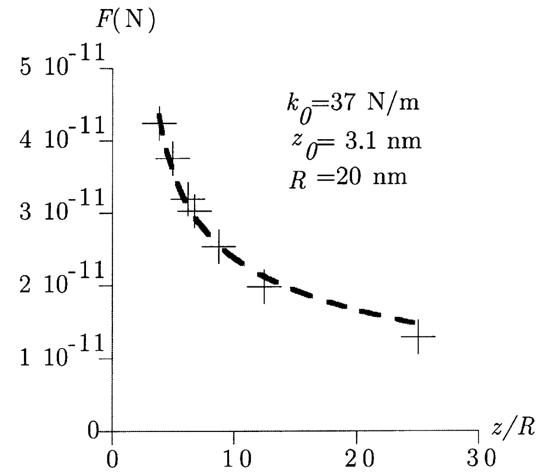

Fig. 5. Experimental data fitted by the approximate force expression.

3 Comparison of the approximate force with experimental measurements and numerical derivations

We have tested expression (9) by comparing its tip-surface dependence with those obtained experimentally and numerically. We have compared the variations of $F_z(z)$ to experimental data obtained by measuring the tip-surface capacitive force between a Pt-coated Si tip and a gold surface. All the experiments are performed under controlled dry gas atmosphere. The geometric tip characteristics ($H = 20\ \mu$m, $\theta_0 = 10°$ and $R = 20$ nm) are determined by electronic microscopy. The tip-surface force is measured using an atomic force microscope in the resonant mode, this allows a precise force determination even far from the surface. In our experiment, the tip is fixed at the end of a cantilever, the tip-surface distance varying over the $(0, 5\ \mu$m) range. A modulated bias voltage $V_1 \sin\omega t$ is then applied between the tip and the gold sample, ω being about 30 kHz. This applied voltage creates a capacitive force F_z on the tip. This oscillating force induces cantilever oscillations which can be measured using optical heterodyne detection. Since the voltage frequency is very far from the cantilever resonance frequency, the vibration amplitude is simply proportional to the applied force. A representative set of data is presented in Figure 5. These force variations can be compared to those obtained using our expression (9) in which $V = V_1$. To fit the data, we must introduce the cantilever hardness k_0. Its value is not known exactly, the cantilever manufacturer giving a hardness of about 50 N/m, and a fit procedure is therefore required. The best fit is obtained for $k_0 = 37$ N/m in agreement with the estimated value. This comparison shows without ambiguity that the force expression obtained in the frame of our model can well describe the experimental data.

Our analytical expression (9) can also be compared to numerical derivations of the tip-surface force obtained for the same tip. The most complete numerical procedure

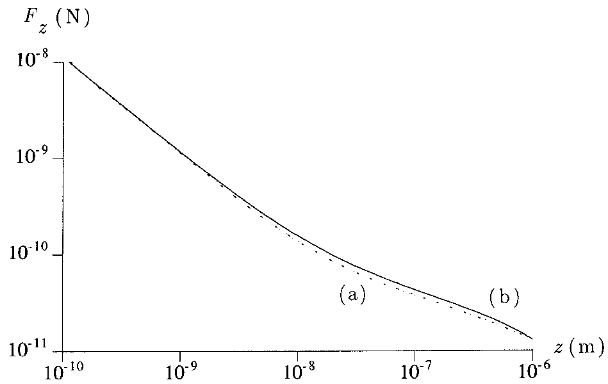

Fig. 6. Comparison between the numerical and analytical variations of the tip-surface force with tip-surface distance z: a) numerical data, b) analytical expression.

used to evaluate this force has been recently proposed by Belaidi *et al.* [6]. In their procedure, they modelled the tip by a series of point charges, their values and positions being calculated to obtain constant potentials on the tip and on the surface. Comparison between their numerical derivation and our analytical evaluation is presented in Figure 6 for a very large tip-surface distance range. The agreement between the two results is good; the difference never exceeding 10%.

Thus, we have developed a very simple method to determine the tip-surface force in Atomic Force Microscopes but this method is more general and can be applied to any axially symmetric capacitor. In this method, the tip is decomposed into infinitesimal surfaces, the infinitesimal contribution being similar to those corresponding to an infinite dihedral capacitor. This assumption is formally valid only if the distance between the conductors is small with respect to their lateral dimensions. Obviously this is not the case for these infinitesimal surfaces for which the edge effects are significant and this assumption should not be used. However it seems that, since we are interested only in global quantities such as the capacitance or the force between the tip and the surface, these effects are compensated and that our approximation does not introduce significant errors. The main advantage of this expression is that it offers the possibility of describing the variation of the force with the tip-surface distance whatever the range whereas the previous asymptotic method does not offer this opportunity.

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