Force on a Conducting Tip near a Metallic Surface Coated with a Polarizable Dielectric Layer: Theory and Experiment*

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In the present study, we have derived a formula for the electrostatic force between the conducting tip and a metallic sample coated with a thin layer of polarizable dielectric of known dielectric constant by exploiting the fact that the tip-sample configuration in scanning probe microscopes can be represented as confocal hyperboloid surfaces of revolution in a prolate spheroidal coordinate system. The general behavior of the dependence of the force on tip-sample separation and the thickness of the dielectric film has been experimentally verified using a conducting atomic force microscope. The results are in better agreement with prolate spheroidal coordinate system over a wide range of tip-sample distances than the results obtained by the widely used sphere-on-plane approximation. [DOI: 10.1380/ejsnt.2011.206]

Keywords: Electric force microscopy; Force-distance curves; Conducting atomic force microscopy

I. INTRODUCTION

From modest beginnings, scanning tunneling microscopy (STM) has been expanded for application to numerous techniques depending on the property used for probing, e.g., magnetic field, electric field, or capacitance, resulting in the development of scanning probe microscopy (SPM) [1, 2]. Knowledge of electric fields in the typical tip-sample configuration is essential for operating the scanning tunneling microscope, the atomic force microscope (AFM), the electric field microscope (EFM), and the other related probe microscopes. A general formula for obtaining the electrostatic potential for conducting tip-sample geometry was developed by Russell [3] using a prolate spheroidal coordinate system [4, 5]. In a previous study, we obtained an expression for the force between the conducting tip and a sample due to the presence of the potential difference as a function of tip-sample distance assuming the geometry of a confocal hyperboloid [6, 7]. The prolate spheroidal coordinate system, which is particularly suitable for the tip-sample geometries used in probe microscopy, is given by

$$\begin{aligned} x &= a[(\xi^2 - 1)(1 - \eta^2)]^{\frac{1}{2}} \cos \phi, \\ y &= a[(\xi^2 - 1)(1 - \eta^2)]^{\frac{1}{2}} \sin \phi, \\ z &= a\xi\eta, \end{aligned} \quad (1)$$

where $1 \leq \xi \leq \infty$, $-1 \leq \eta \leq 1$, and $0 \leq \phi \leq 2\pi$ describe the permissible ranges of coordinates ξ , η , and ϕ , respectively. The tip surface was assumed to be represented by a

portion of the hyperboloidal surface $\eta = \eta_{\text{tip}} = \sqrt{s/(s+R)}$ bounded by the maximum distance r_{max} from the z axis. Here, s is the tip-sample distance, and R is the tip radius. The sample surface is characterized by $\eta = \eta_{\text{sample}} = 0$. In the present paper, we extend these calculations to the estimation of force on the tip when the conducting planar surface is coated with a thin layer of polarizable dielectric of known dielectric constant on the side facing the tip. In addition, it is assumed that this surface can be approximated by a confocal hyperboloid surface of revolution tangent to the dielectric surface at point D (see Fig. 1), that the equipotential surfaces continue to be confocal hyperboloids, and that the electrostatic potential becomes a function of η only. The approximation of treating the plane free surface of the dielectric as a confocal hyperboloid is reasonably good if the thickness of the dielectric layer is sufficiently small, so that significant departure of the hyperboloid from the plane occurs at distances larger than r_{max} as measured from D. Here, r_{max} is the radius at the intersection of bottom of the tip and the surface of the cantilever [6]. In the absence of this cutoff, the expression is logarithmically divergent. Using the notation of Russell, we have

$$a = \sqrt{s(s+R)}; \quad \eta_{\text{tip}} = \sqrt{\frac{s}{s+R}}; \quad \eta_{\text{D}} = \frac{t_{\text{oxide}}}{a}, \quad (2)$$

where 'a' is the focus-sample distance, and t_{oxide} is the dielectric layer thickness at D. The parameters η_{tip} and η_{D} define the surfaces of the tip and the approximating confocal hyperboloid. In the following discussion, the term 'sample' refers to the plane conducting surface, which will be assumed to be at zero potential. The conducting tip will be at a potential of V_b . The Laplace equation reduces to a one-dimensional ordinary differential equation, the general solution of which is of the following form:

$$V(\eta) = A \ln \lambda + B, \quad (3)$$

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FIG. 1: Schematic diagram of the tip-sample geometry used for the calculations.

where

$$\lambda = \frac{1 + \eta}{1 - \eta} \quad (4)$$

and A and B are arbitrary constants. However, the region of interest must be divided into two separate regions such that $\eta_{\text{tip}} \geq \eta > \eta_D$ (Region I) contains free space and $\eta_D \geq \eta \geq 0$ (Region II) contains the dielectric of dielectric constant k . The solution to the Laplace equations $V_1(\eta)$ and $V_2(\eta)$ in Regions I and II, respectively, satisfying the following conditions:

$$V_1(\eta_{\text{tip}}) = V_b; \quad V_1(\eta_D) = V_2(\eta_D) \quad (5)$$

and

$$V_2(0) = 0; \quad V_1'(\eta_D) = kV_2'(\eta_D) \quad (6)$$

are found to be

$$V_1(\eta) = V_b \left(\frac{k \ln \lambda - (k-1) \ln \lambda_D}{k \ln \lambda_{\text{tip}} - (k-1) \ln \lambda_D} \right) \quad \text{Region I} \quad (7)$$

$$V_2(\eta) = V_b \left(\frac{\ln \lambda}{k \ln \lambda_{\text{tip}} - (k-1) \ln \lambda_D} \right) \quad \text{Region II} \quad (8)$$

where

$$\lambda_D = \frac{1 + \eta_D}{1 - \eta_D}; \quad \lambda_{\text{tip}} = \frac{1 + \eta_{\text{tip}}}{1 - \eta_{\text{tip}}} \quad (9)$$

For the purpose of calculating the force on the tip, only the electric field in Region I is needed. The electric field at a point $P(\eta_{\text{tip}}, \xi)$ on the tip surface is given by

$$\vec{E} = \beta_k \left(-\frac{2\alpha}{a} \frac{\hat{\eta}}{\sqrt{(\xi^2 - \eta_{\text{tip}}^2)(1 - \eta_{\text{tip}}^2)}} \right), \quad (10)$$

where

$$\alpha = \frac{V_b}{\ln \lambda_{\text{tip}}} \quad (11)$$

and the factor in brackets is the field at the tip in the absence of a dielectric layer. The effect of the dielectric is incorporated into the factor β_k , which is given as follows:

$$\beta_k = \frac{k \ln \lambda_{\text{tip}}}{k \ln \lambda_{\text{tip}} - (k-1) \ln \lambda_D} \quad (12)$$

so that $\beta_k \rightarrow 1$ when either $k \rightarrow 1$ or $\lambda_D \rightarrow 1$ or when both k and $\lambda_D \rightarrow 1$. Since the calculation of the force on the tip proceeds identically to that undertaken in Ref. [6] for the absence of dielectric layer, the expression for this force when the dielectric layer is present is given as follows:

$$\tilde{F}_z = \beta_k^2 F_z \quad (13)$$

where F_z is the force for a conductor without the dielectric layer [6]. Figure 2A shows the forces on metal and dielectric for confocal hyperboloid geometry. The factor β_k can be compared with the corresponding factor for a planar configuration consisting of two parallel plane conducting surfaces separated by a distance 's' having the parallel plane dielectric layer of thickness ' t_{oxide} ' between the surfaces. This factor is given as follows:

$$\beta_k^{\text{plane}} = \frac{ks}{ks - (k-1)t_{\text{oxide}}} \quad (14)$$

As shown in Fig. 2B, the variations in β_k and β_k^{plane} in Eqs. (12) and (14) increase with the thickness of the dielectric layer.

II. EXPERIMENTAL

The results reported in the present paper were obtained by AFM in non-contact mode using a customized Burleigh AFM head (Metris 2000) in entirely ambient conditions. The electrostatic force measurements were performed using a stylus cantilever constructed of heavily doped Si having a resistivity of 0.01 $\Omega\text{-cm}$ (MikroMasch NSC36). The dynamic in-situ measurement of cantilever dynamics yielded a resonance frequency of 95 KHz and a force constant of 0.45 N/m. The present study focuses primarily on the behavior of the electrostatic force on polarizable dielectric of known dielectric constant. Highly conducting Si(111) of a P-type (resistivity: 0.02 $\Omega\text{-cm}$) wafer with SiO₂ ($k = 4.5$) thicknesses of 25 Å, 50 Å, 80 Å,

FIG. 2: A: Forces on metal and dielectric for $t_{\text{oxide}} = 80 \text{ \AA}$, B: Variations of β_k and β_k^{plane} in Eqs. (12) and (14) with the thickness of the dielectric layer ($V = 8 \text{ V}$, $R = 100 \text{ \AA}$).

and $160 \text{ \AA}$ were used as substrate. Prior to the electrostatic force measurements, samples were investigated by scanning electron microscopy (SEM) and AFM to confirm uniform coverage of SiO_2 . Prior to the experiment, the silica gel was placed in an AFM chamber near the tip-sample assembly in order to avoid the contribution from the residual water layer. Before the non-contact mode experiments, contact mode force curves were obtained in order to estimate the zero points of the X and Y axes, which indicate the tip-sample distance and the force, respectively. These are the points at which the force on the cantilever becomes zero during the approach. The current limiting resistor was used in series with the tip-sample junction to avoid the excessive current flow due to the physical contact between the tip and the sample, which may lead to the modification of the tip/sample surface. The system is then locked in position below the resonant frequency of the cantilever, which is usually performed in non-contact mode for highest sensitivity [8]. The total force on the cantilever in the present case is given as follows:

$$F_{\text{total}} = F_{\text{dc}} + F_0 \sin \omega t, \quad (15)$$

where

$$F_{\text{dc}} = \frac{1}{2} \left(\frac{dC}{ds} V_b^2 \right) \quad (16)$$

and F_0 is the amplitude variation due to cantilever oscillation, and C is the static capacitance. By monitoring the dc shift of the cantilever, it is possible to measure the static deflection of the cantilever as a function of distance. Figure 3 refers to typical force-distance curves at different biases recorded in oscillating cantilever mode. All of the curves in Fig. 3 show two distinct regimes. Far away from the surface the curve varies slowly, which is attributed to the attractive part of the potential. As the cantilever approaches the surface, the behavior changes abruptly from slowly varying to quickly varying at a distance that decreases with the decrease in the bias voltage. In the plot of Fig. 4, in order to eliminate the contribution due to repulsive part of the potential, only the slowly varying part is considered. The tip was positively biased, while maintaining the sample at ground during the experiment. Since the distance between the tip and the sample in non-contact mode is $\sim 200 \text{ \AA}$ or more, high voltage bias

FIG. 3: Typical force-distance curves obtained from the mean deflection of the cantilever at different biases for an oxide layer of $160 \text{ \AA}$ in thickness (taken in dynamic mode)

is required in order to obtain measurable deflection. The dc shift in the detector signal is a measure of the static deflection of the cantilever and is plotted with respect to distance in order to obtain the force curves at constant bias (8 V) for different thicknesses of the dielectric layer.

III. RESULTS AND DISCUSSION

Figure 4A shows the force-distance curves obtained from the mean deflection of the cantilever in dynamic mode for dielectric layers of different thicknesses at constant bias. The figure (inset) clearly shows that the observed force increases with the thickness of the dielectric layer. The thickness dependency of the force curves is shown in the inset of Fig. 4A and obeys $F = kt_{\text{oxide}}^2$ dependence. The experimental results are compared with the theoretical behavior for different tip-sample geometries in Fig. 4B. The data is fitted using the Levenberg-Marquardt method [9] for $r_{\text{max}}/R = 1.9$ and $\chi^2 = 0.98$. The fitted data indicates that the general behavior of the electrostatic force-distance curves for polarizable dielectric is in reasonably good agreement with the experimental data for the range of distances considered in the present study.

FIG. 4: A: Experimental data and data obtained using Eq. (13) for different thicknesses at constant bias. The inset shows a plot of the force with respect to the thickness at constant distance. B: Force curves for metallic tip-insulating surfaces of different geometries ($t_{oxide} = 80 \text{ Å}$, $R = 100 \text{ Å}$, $V = 8 \text{ V}$).

Comparison of the present results with approximations in the literature is instructive. For instance, Hao et al. have studied Coulomb forces by modeling the tip-sample geometry as a sphere-on-flat surface [10]. For the special case of parallel plate approximation of a sphere-plane configuration for very small distances ($R \gg s$) the force can be written as

$$F^{sp} = \pi \epsilon_0 V^2 \left(\frac{R}{s} \right), \quad (17)$$

whereas for larger distances ($R \ll s$) the force can be written as

$$F^{sp} = \pi \epsilon_0 V^2 \left(\frac{R}{s} \right)^2. \quad (18)$$

Figure 4B shows the difference between the confocal hyperboloid and commonly used sphere-plane configuration [11, 12]. The figure shows that in sphere-plane configuration with the condition $R \ll s$ which is relevant to the present work, there is stiff variation in the force for shorter distances and very weak distance dependence for larger distances. However, for the confocal hyperboloid geometry proposed in the present study, the change from long distance to short distance behavior is less abrupt and is in good agreement with the experimental data (Fig. 4A).

Since the radius of the tip is taken as 100 Å , Eq. 17 is not applicable for the data in Fig. 4B.

IV. CONCLUSION

In conclusion, a formula has been derived for the electrostatic force between the conducting tip near a metallic surface coated with a layer of polarizable dielectric. The general behavior of the dependence of the force on tip-sample separation, and the thickness of the dielectric film has been verified experimentally using a conducting atomic force microscope. The results are in better agreement over a wide range of distances, as compared to the commonly used sphere-on-plane approximation.

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