



The contribution of the electrostatic proximity force to atomic force microscopy with insulators

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Abstract

Measurements, using atomic force microscopy, of the force and force derivative on a charged insulating micron sized sphere as a function of gap between the sphere and a conductive plane have revealed attractive forces at finite gaps that are larger than predicted by either van der Waals or conventional electrostatic forces. We suggest that these observations may be due to an electrostatic force that we have identified theoretically and call the proximity force. This proximity force is due to the discrete charges on the surface of the sphere in close proximity to the plane.

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Understanding the electrostatic force of attraction of an insulating sphere to a conductive plane is of importance in many different fields including atomic

force microscopy, semiconductor surface contamination, particle adhesion, and electrophotography. For example, in studies with atomic force microscopes, forces have been observed on charged insulating spheres near conductive planes at finite gaps that are larger than predicted by van der Waals or conventional electrostatic forces. In order to explain these forces unusual localized charge patches or work function anisotropies have been postulated to account for the data [1–3]. The purpose of this Letter is to examine a theoretical model of the attraction of a discrete dis-

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tribution of charge points that are symmetrically distributed around a sphere in contact with a conductive plane [4]. This result is then applied to atomic force microscopy experiments in which forces on charged insulating spherical particles are characterized as a function of the spacing between the sphere and the plane.

It is often assumed in electrostatic calculations that a charged insulating particle can be modeled as a spherically symmetric charge distribution which can be equivalently replaced with a single point charge in the center of the sphere. This is true only in the case of an isolated sphere. It relies on spherical symmetry to apply Gauss' law. However, in the situation in which the quantized nature of the charge is taken into account and the sphere is in contact with a conductive plane, the spherical symmetry no longer exists and no simple integral can be found to apply Gauss' law. Since the conductive plane is an equipotential, the method of images can be used. We use finite element analysis to model the charged insulating particle by a uniform distribution of charge points equally spaced along equally spaced annuli and locate the image charges below the conductive plane by the usual method (see Fig. 1). We will show that the conventional model (which assumes that the charged insulating particle can be replaced by a point charge in the middle of the sphere, even when it is in contact with a conductive plane) underestimates the force of attraction because it ignores the force due to the charges in the proximity of the conductive plane.

We model a charged insulating particle using finite element analysis both analytically and with numerical calculations. The charges are lumped into charge points along a set of N equally spaced annuli parallel to the conductive plane. This allows a derivation of a closed form solution for the electrostatic forces. Assume the charge points are on a sphere of radius R resting on the conductive plane at $z = 0$. The charge points are chosen using polar coordinates to maintain a constant arc length $R\Delta\phi$ between charge points in the two orthogonal directions. The vertical angle between two adjacent annuli, $\Delta\phi$, is given by π/N . Since the circumference of each annulus is different, they each hold a different number of charge points. The number of charge points for the i th annulus is given by

$$k_i = 2N \sin\left(\frac{\pi i}{N} + \frac{\pi}{2N}\right), \quad i = 0, \dots, N-1, \quad (1)$$

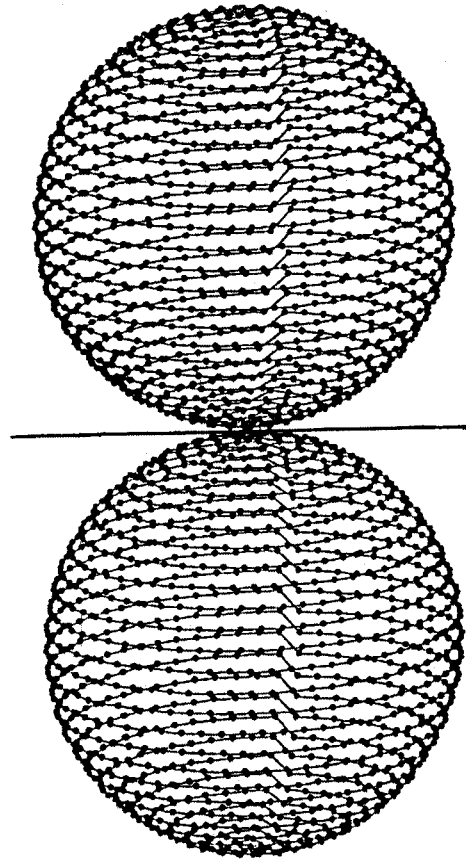


Fig. 1. A sphere with charge points and its image charges. The charge points are arranged along annuli such that the distance between annuli and charge points is the same. For any area on the sphere that includes at least one charge point, the charge per unit area is the total charge on the sphere divided by the total area of the sphere.

where the expression in parenthesis is the latitude angle of annulus i . The $\pi/2N$ term maintains the correct charge density (the total charge Q divided by the area of the sphere) in the tip of the sphere adjacent to the contact point. The total number of charge points, K can be derived by summing the charge points of all the annuli

$$K = \sum_{i=0}^{N-1} k_i = 2N \int_0^{\pi} \sin\left(\frac{\pi x}{N}\right) dx = \frac{4N^2}{\pi} \quad (2)$$

or by dividing the total surface area of the sphere by the area that a charge point occupies, $(R\pi/N)^2$. The charge q in each charge point is the total charge on the

sphere Q divided by K

$$q = \frac{Q}{K} = \frac{Q\pi}{4N^2}. \quad (3)$$

The number of charge points on the first annulus nearest the conductive plane k_0 is given, in the limit for large N , by

$$k_0 = 2N \sin\left(\frac{\pi}{2N}\right) \approx \pi. \quad (4)$$

The plane of the i th annulus crosses the z -axis at

$$z_i = R \left[1 - \cos\left(\frac{\pi}{2N} + \frac{\pi i}{N}\right) \right], \quad i = 0, \dots, N-1. \quad (5)$$

Using the first two terms of the Taylor series expansion, the separation z_0 of the first annulus from the reference plane $z = 0$ is given by

$$z_0 = \frac{R}{2} \left(\frac{\pi}{2N}\right)^2. \quad (6)$$

Consider the electrostatic forces due to the interactions between the charge points located in proximity to the conductive plane (which are on the first annulus) with their image charges located symmetrically across the conductive plane. Using Coulomb's law, the force on a single charge point q in the first annulus due to its own image charge point F_{11} (the attractive forces can be expressed by the elements of a rank 2 matrix $[F_{ij}]$, where index i refers to a charge point in an annulus and index j refers to an image charge point) located symmetrically across the conductive plane can now be derived, using Eqs. (3) and (6), in a closed form by

$$F_{11} = \frac{1}{4\pi\epsilon_0} \frac{q^2}{(2z_0)^2} = \frac{1}{4\pi\epsilon_0} \frac{Q^2}{(2R)^2} \frac{4}{\pi^2}. \quad (7)$$

Note that the functional dependence of q and z_0 on the number of annuli N as given by Eqs. (3) and (6) cancels out. Since there are approximately π charge points in the first annulus (Eq. (4)), the contribution to the electrostatic force by these charges, which we will call the proximity force F_p is:

$$F_p = \pi F_{11} = \frac{1}{4\pi\epsilon_0} \frac{Q^2}{(2R)^2} \frac{4}{\pi}. \quad (8)$$

This is a remarkable result. Only a few point charges with a fractional charge q , which are located in the vicinity of the contact point, can generate an attractive

force 1.27 (i.e., $4/\pi$) times greater than a charge Q located at the center of sphere. We note that this result is independent of the number of annuli, N , in the limits of large N .

In principal, all of the other image charges contribute to forces on the charges in the first annulus, which are identified as F_{12} , F_{13} , etc. However, for a large N , the separation $2z_0$ is small compared to the distance to all other charge points. The closest image charges are those due to the charges in the second annulus (z_1) which are easily shown to have negligible contributions since $z_1/z_0 = 9$.

Since the number of point charges considered in the proximity annulus is much smaller than the total number of charge points, i.e., $k_0 \ll K$, the rest of the charge points can still be considered as a complete sphere of charge. This can be modeled by the usual method of placing a single charge in the center of the sphere, giving for the force for the bulk of the charges F_b

$$F_b = \frac{1}{4\pi\epsilon_0} \frac{Q^2}{(2R)^2}. \quad (9)$$

The total electrostatic force F is sum of the electrostatic forces due to the bulk of the charges Q (Eq. (9)) and the proximity charges (Eq. (8)),

$$F = F_b + F_p = \frac{1}{4\pi\epsilon_0} \frac{Q^2}{(2R)^2} \left(1 + \frac{4}{\pi}\right), \quad (10)$$

which has a new factor $(1 + 4/\pi)$, compared to the conventional result (Eq. (9)). This simple derivation shows that a closed form solution for the electrostatic force of a discrete distribution of charge points that are symmetrically distributed around a sphere in contact with a conductive plane can be derived in a straightforward way and provides a useful and universal result that allows a physical interpretation of the $4/\pi$ term.

A numerical calculation was carried out to support the analytical derivation of the electrostatic proximity forces. As before, the assumption is made that the charge on the surface of a insulating sphere can be lumped into K charge point. Two parameters were varied, the number of annuli N and the separation s between the bottom of the sphere and the conductive plane. The force of attraction is given by the double sum of the force of attraction of all the charge points

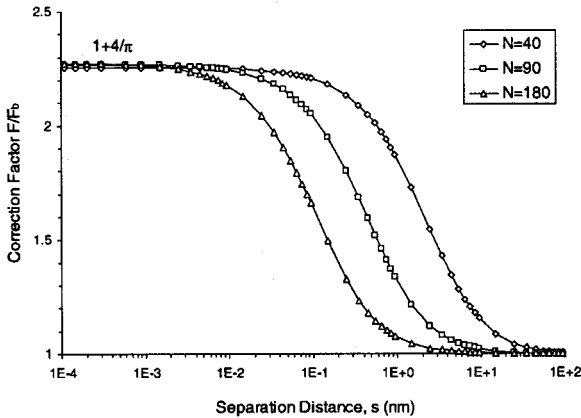


Fig. 2. Correction factor to the electrostatic force normalized to F_b vs. log of the separation distance s between the sphere and the conductive plane, and N , the number of annuli, for a 6 micron radius sphere.

to all of the image charges

$$\vec{F} = \frac{1}{4\pi\epsilon_0} \sum_i^K \sum_j^K q_i q_j \frac{\vec{r}_i - \vec{r}_j}{|\vec{r}_i - \vec{r}_j|^3}. \quad (11)$$

Index i is assigned to the point charges and the index j assigned to the image point charges. The position vectors \mathbf{r} define the location of the charge points from the center of a Cartesian coordinate system coinciding with the contact point. The image force F in Eq. (11) can be normalized with the bulk force F_b , giving F/F_b which we will call the correction factor. The correction factor is plotted against the separation distance s in Fig. 2 for the number of annuli $N = 40, 90$ and 180 . At a separation distance s larger than 50 nm, the electrostatic force exerted on a uniformly charged sphere is well represented by the conventionally assumed value (Eq. (9)), i.e., the correction factor is equal to one. On the other hand, at a separation distance s smaller than 50 nm, Eq. (9) does not equal to the total electrostatic force and the ratio F/F_b diverges from the ratio of 1 at a rate depending on the number of annuli N , which determines the precise locations of the point charges. However, all force curves converge to the same value $(1 + 4/\pi)$ at contact, independent of the number of annuli. This result is in excellent agreement with the general analytical result, Eq. (10).

This correction factor has interesting mathematically characteristics. Depending on the order in which N goes to infinity (which represents a uniform distrib-

ution) and s goes to zero, the correction factor goes to either 1 or $1 + 4/\pi$. However, for any finite N , the correction factor goes continuously to $1 + 4/\pi$ at $s = 0$ as the gap is reduced (see Fig. 2). Physically only finite N is meaningful because charge is quantized. For the example in Fig. 2 (which assumes a 6 micron diameter particle) for $Q = 12$ fC at $N = 180$ there are 41 000 charge points and 2 electrons per charge point. z_0 (Eq. (6)), the distance from the charge point to the conductive plane, is 0.23 nm.

The gap at which the proximity force can be detected can be derived. Note from Fig. 2 that values of s at which this new proximity force is measurable depends on the assumptions in the model, i.e., the number of annuli assumed. This suggests that the observation of this force as a function of gap will depend on the details of the actual charge distribution in the proximity of the contact. If we assume the proximity force can be observed when it is 10% of the bulk force, then it is easily shown (by replacing z_0 in Eq. (7) with $z_0 + s_{10}$ and equating this to π times this force to 0.1 times Eq. (9)) that the gap s_{10} at this point is

$$s_{10} = \left(\sqrt{\frac{40}{\pi}} - 1 \right) \frac{R\pi^2}{8N^2}. \quad (12)$$

Using Eq. (2), this becomes

$$s_{10} = \frac{R}{K} \left(\sqrt{\frac{40}{\pi}} - 1 \right) \frac{\pi}{2} = 4.0 \frac{R}{K}. \quad (13)$$

Noting that charge is quantized so that N is finite and K cannot be larger than Q/e , where e is the electronic charge, the minimum s_{10} is $4Re/Q$. This is 0.32 nm for a uniformly charged particle with radius of 6 microns and charge of 12 fC but is 32 nm for the same particle charged with clusters of 100 electrons per charge point. (Strictly speaking, Q can be a fraction of e which occurs in some semiconductor surface electronic charge distributions.) By comparing s_{10} to z_0 it can be seen that the proximity force is active (equal to 10% of the conventional force) at gaps approximately equal to the spacing between the charge and the ground plane if the charges are uniformly distributed on the surface of the sphere. A non-uniform distribution significantly increases the range of the proximity force.

These results are valid even if the distribution of charge points is changed. The charge point distribution that we chose gives a good estimate of the prox-

imity force, independent of the detailed distribution of the charge points. For $N = 180$ (Fig. 2), there are 2 electrons (q) in each of the π charge points spaced (z_0) 2.3 Å from the conductive plane. Another distribution, which one might think maximizes this proximity force, could be constructed by starting with one electron positioned at the point of contact between the sphere and the plane. Using Eq. (9) to quantify this force, and using a reasonable semi-classical estimate of the closest approach of two materials, 2.5 Å, giving $z_0 = 1.25$ Å (used to estimate the magnitude of the van der Waals forces in standard solid state textbooks [5]), this proximity force is actually less; it would be comparable only at $z_0 = 0.65$ Å.

We have shown both analytically and numerically that the electrostatic force on a charged insulating sphere in contact with a conductive plane has two components: (1) one due the bulk charges which can be calculated by replacing the charged sphere with its charge in its center and (2) a newly derived component due to the charges in proximity to the plane which is larger than the bulk force component by a factor $4/\pi$. The fact that our result is independent of the details of the model, i.e., the number of annuli or the detailed distribution of the charge points, suggests that this result describes an additional electrostatic force on any charged insulating particle which has not been identified previously. Further, we can physically identify the source of the proximity force: it is due to the charges in closest proximity to the contact point.

The gap s at which this new proximity force is measurable depends on the number of annuli assumed (Fig. 2), i.e., the details of the charge distribution model in the vicinity of the contact. Conversely, the shape of the force function in the pre-contact region for a separation distances less than 50 nm may give an important clue about the magnitude and the distribution of charges in the proximity of the contact point. For example, a sharp increase of force by a factor $1 + 4/\pi$ within a few tenths of a nm prior to contact (consistent with Eq. (13)) might indicate a very uniform surface charge density. Alternatively, an experimental observation of a force increase at much larger separations (such as observed in Refs. [1–3], see below) might be interpreted as a uniform distribution of clusters of the elementary electronic charge.

In a series of papers Gady et al., e.g., Refs. [1,2], and others [3,6,7] have convincingly shown in atomic

force microscopy measurements using charged insulating particles that are brought into close proximity with a conductive plane, that there exists an attractive force between the insulating particle and a conductive plane that is larger than predicted by van der Waals or conventional electrostatic forces at finite gaps. Prior attempts to understand these results required postulating unusual localized charge patches [1,2] or work function anisotropies [3] whose parameters could not be independently verified. For example, Ref. [1] describes force microscopy with charged polystyrene spheres. To account for these data a localized charge patch with a charge density σ of approximately 80 nC/cm² was assumed to be created by prior contacts at the contact region, despite the fact that this particle was already charged (with a charge density of 1 nC/cm²). We are pointing out that there is no need to assume a localized charge patch that has never been directly observed on an already charged particle. The proximity force discussed here can account for these data. In Fig. 3(a) of Ref. [1] the van der Waals force can quantitatively account for the data at gaps less than 10 nm. But at and above 20 nm, the observation is larger than can be accounted for by either van der Waals or conventional electrostatic forces (Eq. (9)). But as can be seen in our Fig. 2, at 20 nm there are significant contributions to the force (and force derivative) by the proximity force which exceeds the contribution due to Eq. (9), with the magnitude depending on N , the number of annuli assumed, i.e., the charge distribution, and the charge on the particle.

Quantitative comparison of the data given in Ref. [1] and the proximity theory (derived from tables of values from which Fig. 2 is plotted to obtain the derivatives) gives values close to the values observed in Fig. 3(a) and (b) of Ref. [1] and, perhaps more significantly, reproduces the change in observed force derivative as the gap is changed for reasonable values of the parameters. At 20 nm, based on Eq. (8) and Table I from Ref. [1], we estimate the van der Waals force derivative is 2×10^{-6} CV/cm². The conventional electrostatic force (our Eq. (9)) is 2×10^{-8} CV/cm², much too small, as the authors pointed out. Another force is needed to account for the data. We estimate the proximity force derivative at $N = 40$ is 1.3×10^{-7} CV/cm² at 20 nm for the charge per unit area given. Actually this corresponds

to a charge to mass ratio of only $8.3 \mu\text{C/g}$ for a 6 micron particle, a very unusual low value. If the charge is assumed larger by a factor of 4, the proximity force derivative exactly matches the observed data. Even more significant, the data indicates that the observed force derivative decreases by about a factor of 3 from gaps of 20 to 32 nm. The proximity force derivative decreases by exactly this amount (independent of the absolute value of the charge).

Experiments in which both the force and force gradient between a 3 micron diameter polystyrene sphere and a grounded highly oriented pyrolytic graphic substrate were reported by Gady et al. in Ref. [2]. Again a localized charge patch is postulated to account for the force data which are observed to be larger than can be accounted for by van der Waals forces or by Eq. (9) at finite gaps. As the total charge on the polystyrene sphere is not reported, quantitative comparison of the data with the proximity force cannot be done. But the close resemblance of the data to the data of Ref. [1] suggests that the proximity force also can account for these data. In addition, the authors themselves recognize that the localized charge patch model has a significant “dilemma” (to use their word): the electric field $\sigma/2\epsilon_0$ due to the postulated localized charge patch ($500 \text{ V}/\mu\text{m}$) exceeds the electric field that air can support by an enormous factor, roughly 170 (using the usual value for Paschen breakdown of $3 \text{ V}/\mu\text{m}$ for macroscopic distances). Accounting for the data with the proximity force eliminates this dilemma.

There are many other examples in the literature of atomic force microscopy involving insulators, of the observation of unexplained forces which the proximity force could explain. For example, in Ref. [3], measurable attractive forces are observed between a nominally uncharged 300 nm diamond tip and a graphite surface as far away as 4 nm. Van der Waals attractive forces, using well established parameters, cannot account for a measurable attractive force beyond about 0.4 nm in these experiments. Work function anisotropies were suggested as the origin of these long range forces. The experimentally observed attractive force reported in Ref. [3] is just in the range that the proximity force is observable, assuming a uniform distribution of charges on the diamond tip and estimates based on Fig. 2 or Eq. (13). As is well known, it is very difficult to eliminate charges from an insulating

surface, which can be charged by contact with any other material throughout its history. For another example, in Ref. [8], it is stated that “we also detected a weak component of the short-range force exhibiting a longer decay length than expected for purely covalent forces”. The proximity force could account for this observation also.

This proximity force also contributes to charge particle adhesion, i.e., attractive forces at zero gap, and in some cases can dominate van der Waals forces. The proximity force needs to be added to the usual electrostatic and van der Waals forces [9]. Since real particles have many contact points with a plane and at each contact point the proximity force can be active, the proximity force can dominate the other forces of adhesion. Ref. [9] describes such a situation.

In conclusion, an electrostatic force has been identified, which we have called the proximity force. It is due to the discrete charges on the sphere which are in close proximity to the contact plane. In contact with a conductive plane, a discrete distribution of charge points that are symmetrically distributed around a sphere has a proximity force equal to $4/\pi$ times the conventional force. At finite gaps, the attractive force between a charged insulating particle and a conductive plane, as revealed in atomic force microscopy measurements, is larger than predicted by van der Waals or conventional electrostatic forces. This proximity force can account for these data.

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