Potential distribution and field intensity for a hyperboloidal probe in a uniform field

A. Passian and A. Wig
Oak Ridge National Laboratory, Photometrics Group, Life Sciences Division, Bethel Valley Road, Oak Ridge, Tennessee 37831-6123

F. Meriaudeau
Université de Bourgogne, IUT du Creusot, Le2i, 12 rue de la Fonderie, 71200 Le Creusot, France

T. L. Ferrell
Oak Ridge National Laboratory, Photometrics Group, Life Sciences Division, Bethel Valley Road, Oak Ridge, Tennessee 37831-6123 and Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996-1200

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The scalar potential and electric field distributions in the gap region of a probe-substrate system are calculated. The probe, modeled as a dielectric medium with the geometry of a one-sheeted hyperboloid of revolution, is located above a charged substrate surface which is modeled as a dielectric half space interfaced with a uniform surface charge density. The potential and field distributions are then calculated as functions of the dielectric constant of the medium filling the space between the tip and the surface, and as functions of the hyperboloidal shape parameter. Comparisons are made with the case of a dielectric spheroidal body. The analytical results attained can be used to study other related quantities such as energy density or Coulomb interaction in the neighborhood of the nanometer sized apex region without resorting to numerical methods. This investigation allows for tip shape related field variation in various dielectric media to be studied.

Application of this approach to modeling probe tip-sample (probe tip-substrate) interaction in scanning probe microscopy, or to modeling dielectric breakdown processes, are examples of the potential use of the method. © 2002 American Vacuum Society. [DOI: 10.1116/1.1428268]

I. INTRODUCTION

A knowledge of the behavior and the electric properties of various gaseous or liquid dielectric media can be gained by studying the response of such media to an applied electric field. In situations where the geometrical pattern of the established field plays an important role, special care must be taken in the analysis and evaluation of the relevant quantities in the neighborhood of the surfaces involved. The material interfaces or the surfaces bounding the material domains, depending on the particular geometry, are typically approximated in an appropriate coordinate system with surfaces represented by a constant coordinate. Several authors have studied such material interfaces where the dielectric function of the system experiences a discontinuity. Becker et al. studied the resonant surface modes for a hyperboloidal void to model a submicron hole in a dielectric material under the assumption of a local dielectric function for the medium. Similarly, Ferrell calculated the nonretarded surface plasmon dispersion relations for several cases related to scanning probe microscopy where the material domains were modeled as hyperboloids of revolution.

Here we consider the case of a hyperboloidal dielectric tip immersed in a homogeneous field set up by a uniform surface charge density residing on a plane bounded semi-infinite dielectric medium. The problem is modeled in a prolate spheroidal coordinate system, where the hyperboloidal probe and the Cartesian substrate surface can be naturally represented each as a surface of constant coordinate. An advantage of this geometry is that the solutions can be obtained analytically, and having explicit expressions for potential and field quantities are of great importance to many applications such as in scanning probe microscopy. In the event that a multilayer structure with hyperboloidal geometry including dispersive media with complex dielectric functions is of interest, the approach here can be useful, in particular for the study of thin film behavior in the apex region. This is especially interesting for time dependent problems where retardation effects can be ignored due to the subwavelength apex region. The dielectric media considered in this work are linear, isotropic, and homogeneous. By letting the dielectric constant of the tip tend to large values, we can, using this approach, simulate the metallic tip limit.

A short background is given in Sec. II, where the details concerning the solutions to the Laplace’s equation in prolate spheroidal coordinate system are discussed. The analytical expressions for the field components and corresponding equipotential surfaces are obtained in Sec. III, for the case of azimuthal symmetry. Here specifying the index of refraction of the material in which the field intensity is sought explicitly influences the results. The numeric evaluation of these results, summarized in Sec. IV, involves evaluations of infinite double integrals similar to those arising in Mehler–Fock integral transforms with the conical functions as the kernel. In Sec. V we discuss the results and include a conclusion.
II. BACKGROUND

Cartesian and Spheroidal coordinate systems are connected via

\[ \begin{align*}
  x &= z_0 \sin \xi \sin \theta \cos \varphi = z_0 \sqrt{(\eta^2 - 1)(1 - \mu^2)} \cos \varphi, \\
  y &= z_0 \sin \xi \sin \theta \sin \varphi = z_0 \sqrt{(\eta^2 - 1)(1 - \mu^2)} \sin \varphi, \\
  z &= z_0 \cosh \xi \cos \theta = z_0 \eta \mu,
\end{align*} \]

where the spheroidal variables are defined in the ranges \( 0 \leq \xi < \infty, \ 0 \leq \theta \leq \pi, \) and \( 0 \leq \phi < 2 \pi. \) The variable substitutions \( \cosh \xi = \eta \) and \( \cos \theta = \mu \) have been made in writing the right-hand side of Eq. (1). The scale factor \( z_0 \) defines the focal distance of the confocal hyperboloids spanning the left-hand side of Eq. (1) for fixed \( \mu \) with the corresponding orthogonal, confocal prolate spheroids for fixed \( \xi. \)

The scalar electric potential for the particular geometry of a hyperboloidal dielectric tip considered here, shown in Fig. 1, is obtained by solving Laplace’s equation in prolate spheroidal coordinates \((\xi, \theta, \varphi)\) system. Utilizing the complex separation constant \(-\frac{1}{2} + iq\), where \(q \in [0, \infty]\) is real and continuous, Laplace’s equation in this coordinate system is separated, resulting in real eigenvalues \((q^2 + \frac{1}{2})\), and eigenfunctions with a continuous spectrum. The resulting differential partial equations are satisfied by the conical functions \( P_{1/2+iq}^m(\xi) \) with an argument \(\xi \in ]-\infty, \infty[\). Superposition in the variable \(q\), in terms of infinite integrals, composes the general solution for each azimuthal mode.\(^5\)

The general solution to the Laplace’s equation, for the present case of azimuthal symmetry, involves superpositions of linear combinations of conical functions \(P_{1/2+iq}^m(\pm x)\) only, where \(x = \cos \theta \) or \(x = \cosh \xi \) depending on the particular solution in the respective spheroidal variable.\(^4\)

III. POTENTIAL AND FIELD DISTRIBUTION

The scalar potential corresponding to the solution of the Poison’s equation, for the configuration given in Fig. 1, is assumed to be given by the following general form:

\[ \Phi(\vec{r}) = \Phi_1(\vec{r}) \Theta(\theta_1 - \theta) \Theta(\theta - \theta_1) \Theta\left(\frac{\pi}{2} - \theta\right) + \Phi_2(\vec{r}) \Theta(-\xi), \]

where \(\Theta(\theta)\) is the Heaviside’s step function, and \(\Phi_i\) are the solutions to Laplace’s equation. The dielectric constants for the tip and the substrate regions have been set to \(\varepsilon = \varepsilon\) and \(\varepsilon = \varepsilon\), respectively, while for the region between the tip and the substrate it has been taken as \(\varepsilon = 1\), without any loss of generality. We assume real and frequency independent dielectric functions for the involved media. Incorporating the continuity of the potential everywhere and the discontinuity of the normal component of the displacement field at \(\mu = 0\), due to the surface charge density \(\sigma\), we write the partial potentials \(\Phi_i(\vec{r})\), \(i = 1, 2, 3\), in terms of the following infinite integral:

\[ \Phi_i(\vec{r}) = (4\pi \sigma z_0) \int_1^\infty \varphi_{q,i}(\eta, \eta', \mu) \eta' d\eta', \]

with \(\varphi_{q,i}\) given by

\[ \varphi_{q,i}(\eta, \eta', \mu) = \int_0^\infty U(q) \varphi_i(\mu) \times P_{1/2+iq}(\eta) P_{1/2+iq}(\eta') dq, \]

and \(\varphi_i(\mu)\) given by

\[ \begin{align*}
  \varphi_1(\mu) &= \beta_q(\mu_i) P_{1/2+iq}(\mu), \\
  \varphi_2(\mu) &= P_{1/2+iq}(\mu) - \alpha_q(\mu_i) P_{1/2+iq}(-\mu), \\
  \varphi_3(\mu) &= (1 - \alpha_q(\mu_i)) P_{1/2+iq}(-\mu),
\end{align*} \]

where \(\alpha_q(\mu_i)\) and \(\beta_q(\mu_i)\) are continuous, and well-behaved functions of \(q\) and the tip shape \(\mu_i = \cos \theta_i\), and are given by

\[ \begin{align*}
  \alpha_q(\mu_i) &= \left(\frac{\varepsilon - 1}{\varepsilon - \varepsilon_q(\mu_i)}\right) K(\mu_i), \\
  \beta_q(\mu_i) &= \left(\frac{\varepsilon - \varepsilon_q(\mu_i)}{\varepsilon - \varepsilon_q(\mu_i)}\right).
\end{align*} \]

with \(K(\mu_i) = P_{1/2+iq}^0(\mu_i) / P_{1/2+iq}^0(-\mu_i)\) and \(K'(\mu_i)\) being the corresponding ratio of their partial derivatives with respect to \(\mu\), that is, after simplification

\[ K'(\mu_i) = - \frac{P_{1/2+iq}^0(\mu_i)}{P_{1/2+iq}^0(-\mu_i)} \]

and \(\varepsilon_q(\mu_i) = K(\mu_i) / K'(\mu_i).\) We note here that, due to the properties of the conical functions in the limit of vanishing argument, \(K'(0) = -1\). The common amplitude \(U(q)\) in Eq. (4) is given by

\[ U(q) = \frac{\pi \tan \pi q}{\pi q \cosh \pi q} f(q) P_{1/2+iq}(0), \]

with \(f(q)\), which characterizes the degree of polarization of the dielectric medium of the probe, given by

\[ f(q) = \frac{1}{(1 + \varepsilon) + (1 - \varepsilon) \alpha_q(\mu_i)}. \]

By considering the asymptotic expansions\(^6\) of the involved functions in Eq. (6), one can show that...
\[ e_r(\mu_i) \to -1, \quad q \to \infty \]  

and thus
\[ \alpha_q(\mu_i) = e^{i(2 \theta_i - \pi)} \to 0, \quad q \to \infty \]  

\[ \beta_q(\mu_i) = \frac{2}{1 + \varepsilon}, \quad q \to \infty \]  

as \( 2 \theta_i - \pi < 0 \) is always fulfilled for any physically realistic probe shapes. Similarly, we observe that
\[ U(q) \approx \frac{\sqrt{2} \pi}{(1 + \varepsilon)} q^{3/2} e^{-(1/2)q} \to 0, \quad q \to \infty \]  

\[ f(q) = \lim_{q \to \infty} f(q) + g(q), \quad q \to \infty \]  

\[ = \frac{1}{1 + \varepsilon} + g(q). \]  

These limiting considerations allow us to write the potential in the region between the tip and the substrate as
\[ \Psi_2(\rho) = -\eta \mu \left( \frac{1}{1 + \varepsilon} + \int_1^\infty \eta' d\eta' \right) \]  

\[ \times \int_0^\infty D_\mu(q) P_{-1/2+iq}(\eta) P_{-1/2+iq}(\eta') dq, \]  

where we have introduced the following notation for convenience:
\[ D_\mu(q) = h_1(q) d_{1,\mu}(q) + h_2(q) d_{2,\mu}(q) \]  

and
\[ h_1(q) = w(q) g(q) P_{-1/2+iq}(0), \]  

\[ h_2(q) = w(q) f(q) \alpha_q(\mu_i) P_{-1/2+iq}(0), \]  

\[ d_{1,\mu}(q) = P_{-1/2+iq}(\mu) - P_{-1/2+iq}(-\mu), \]  

\[ d_{2,\mu}(q) = P_{-1/2+iq}(0) - P_{-1/2+iq}(-\mu), \]  

with \( w(q) \) defined by
\[ w(q) = \frac{\pi q \tanh \pi q}{\cosh^2 \pi q}. \]  

We also note that in the final form of Eq. (15), we have assumed for simplicity that the dielectric constant of the probe material is identical to that of the substrate. It can be seen that the material properties of the probe are expressed explicitly by Eq. (14). Thus, any limiting considerations, such as \( \varepsilon \gg 1.0 \) regarding the metallic tip limit, must rely on the behavior of
\[ f(q) = \frac{1}{1 + \alpha_q(\mu_i) + \varepsilon[1 - \alpha_q(\mu_i)]}. \]  

Finally, the electric field corresponding to the potential in Eq. (15) can be written as
\[ E_2(\rho) = \frac{2 \pi \sigma}{\sqrt{\eta^2 - \mu^2}} \left\{ \mu \sqrt{\eta^2 - 1} \eta \sqrt{1 - \mu^2} (0) + 2 (I_\eta, I_\mu, 0) \right\}, \]  

where the first term on the right hand side is the limiting potential in the limit when the dielectric functions of the system approach 1. The integrals on the right-hand side of Eq. (19) are given by
\[ (I_\eta, I_\mu, 0) = \int_0^\infty \eta' dq \times \int_0^\infty \left( -D_\mu(q) P_{-1/2+iq}(\eta) \cdot H_\mu(q) \right) \times p_{-1/2+iq}(\eta') dq, \]  

where we have defined \( H_\mu \) as
\[ H_\mu(q) = h_1(q) P_{-1/2+iq}(\mu) + h_2(q) P_{-1/2+iq}(-\mu). \]  

As a validation check, we observe that as the dielectric vanishes, i.e., \( \hat{\varepsilon} \to 1 \), we have \( \alpha_q(\mu_i) \to 0 \) and \( h_2(q) \to 0 \), which in turn results in \( E(\rho) \to E_0(\rho) \) and thus the field reduces properly to the case of a uniform surface charge density only with no polarizing media present.

IV. RESULTS

We confine our simulations to the apex region of the probe where the variation in curvature of the modeling hyperboloid is largest. The simulated quantities constituting the potential equation (15), and the field equation (19), both given in Gaussian units, indicate that the tip shape dependency is confined to the region where tip curvature variation is non-negligible as a function of \( z \). For the tip angles in the range \( 0.17 \leq \theta_i \leq 0.65 \) considered, the variation in the curvature of the tip is less than 3.6% for \( \zeta \) as low as 2.0.

The numerical work involves the evaluation of the conical functions in the appropriate range of their parameters and arguments and the evaluation of the infinite double integrals in \( q \) and \( \eta \). The conical functions with argument \( \eta = \cosh \zeta \) oscillate strongly with \( q \) and \( \zeta \). For moderate values of \( q \) and \( \zeta \) these functions were evaluated using their integral representations, whereas for large \( q \) or for not too large \( q \) but large \( \zeta \) and \( \theta_i \), an asymptotic expansion in terms of Bessel functions \( 10,11 \) was used. All the values attained in our simulations were, within the scope of the reported data, in agreement with Refs. 12, 13, and 11.

The scalar potential in the neighborhood of the apex is found by explicit simulation of Eq. (15). A five-point Newton–Cotes algorithm \( 14 \) was employed in order to perform the numerical integrations. In what follows, we have assumed a surface charge density \( \sigma = 1/4 \pi \varepsilon_0 \) (or \( \sigma = \varepsilon_0 / \varepsilon_0 \) in SI units) for convenience, as this sets the constant \( 4 \pi \sigma \varepsilon_0 \) in Eq. (15) to unity.
For a tip angle of $\theta_i = 0.2 \text{ rad}$ and an observation window defined by the coordinates $\theta_i$, and $\zeta_i$ in the ranges $\theta_i = \theta_i = \pi/2$, and $0.0 \leq \zeta_i \leq 2.0$, and increments of $\Delta \theta_i = 0.032$ and $\Delta \zeta_i = 0.020$, the result is shown in Fig. 2. The horizontal and vertical dimensions in this figure have been converted to the Cartesian coordinates for illustration purposes. It should be noted that the metric units of the $x$ and $z$ axes are absorbed in $z_0$, and thus any units associated with $z_0$ will inherently determine the physical size of the examined region. This is a property of the employed coordinate system. The $x$ axis is the radial distance $R$ compiled from Eq. (1) for the given observation interval. The calculation assumes a probe and substrate dielectric constant of $\varepsilon = \varepsilon = 2.13$, and a free space gap dielectric constant $\varepsilon = 1.0$. The dielectric constants can be adjusted to experimental or theoretical values of interest. The values of the potential given in Fig. 2 are in units of volts and are for a focal distance $z_0 = 100.0 \text{ nm}$ and a charge density of $\sigma = 8.8 \text{ nC/cm}^2$. This is a typical value for the charge densities involved in scanning probe microscopy experiments. For example, in atomic force microscopy experiments, sample surfaces can be charged (naturally or by applying a small potential difference between the cantilever and the substrate surface) with densities ranging from several $\mu\text{C/cm}^2$ down to $\text{pC/cm}^2$.

In Eq. (15) a mesh of $\Delta \varphi_i = 0.01$ generates a small enough increment to display smoothly the behavior of the integrand, and a source mesh of $\Delta \zeta_j = 0.01$ was used to perform the integration in the source coordinate $\zeta$.

As can be seen from Fig. 2, the projection of the equipotential surfaces on the $\varphi = 0$ plane are lines which, in the vicinity of the $x = 0$ substrate surface, are parallel to the $x\text{-}y$ plane, while the influence of the polarized dielectric probe tip causes the lines to undergo a curvature proportional to the curvature of the probe and the strength of its dielectric constant. The higher the refractive index of the tip, the higher the curvature of the corresponding equipotential surfaces.

Here, for comparison purposes, we simulate the equipotential surfaces of the scalar potential, and the magnitude of the field, in the interior and the exterior region for a dielectric spheroid in a uniform field. Figure 3 displays the equipotential surfaces. It can be seen in both Figs. 2 and 3 that the effect of the polarized dielectric material diminishes away from the medium in the lateral direction. For the infinite hyperboloidal medium, however, the potential is modified in the vertical direction and close to the boundary of the material. Obviously, the electric field lines are traces of perpendicular direction to the equipotential surfaces.

Similarly, the magnitude of the electric field as given by Eq. (19) was simulated for a tip and substrate dielectric constant $\varepsilon = \varepsilon = 4.0$ in the same free space observation region as before. Figure 4 displays the loci of constant field magnitude. As can be seen, the constant field magnitude here forms a dipole-like pattern around the extremity of the probe, whereas horizontally away from the probe apex, the loci tend to become parallel. In the spheroidal case these loci are depicted in Fig. 5, where, due to the finite material domain of the spheroid, they form closed loops. The influence of the hyperboloidal curvature, as opposed to that of the spheroid, on these patterns is evident from these figures.
V. CONCLUSION

We conclude from the results presented here that the analytical approach employed in this work offers an explicit way to study the effects of the probe material and shape on the potential distribution and the field pattern in the gap region, or to study the effects of a particular gap or substrate material on the field. The results can be applied to scanning probe microscopy studies where a knowledge of the Coulomb interaction of the probe with the sample surfaces is important, for example when calculating the energy or force density inside the probe or in the region between the probe and another dielectric or metal interface. The displayed geometric differences in the field pattern for the hyperboloidal and spheroidal systems are important. In particular, in nonstatic cases in which dispersion is significant the continuum of wave vectors associated with hyperboloidal solutions is far more physical than the discrete spectra offered by the spheroidal solutions. Using this approach, the authors are currently involved in calculating the coupling of optically excited surface plasmons in a hyperboloidal configuration in order to enhance the signal-to-noise ratio in certain types of photon scanning tunneling microscopes (PSTMs).

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