Electric Potential and Field Near Pointed Shaped Surfaces

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Abstract: The trajectories of charged particles, emitted from within or from the close vicinity of pointed shaped surfaces, requires the knowledge of the electric field resulting from the potential bias between surface and detector, or screen. Frequently it is necessary the use of numerical methods for solving Laplace's equation as a result of difficulties in obtaining an analytical expression. Recently we have shown that, when any two coordinate surfaces of an orthogonal system are kept at two different but constant potentials, it is possible to obtain an analytical solution for the potential in a relatively simple manner. Using this general property of orthogonal coordinate systems, we present the solution for the electric potential and field in the vicinity of pointed surfaces for several cases of practical interest in field emission, field ionisation, atom-probe field ion spectroscopy and related phenomena.

1. INTRODUCTION

The adequate modelling of the surface geometry, electric potential and field in the region close to the sample in the Field Ion Microscope (FIM) and in the Field Emission Microscope (FEM) is an important procedure in determining quantities related to tunnelling probabilities as well as the trajectories of the charged particles, ions or electrons. To properly deal with this we have to consider two different aspects: i) the overall variation of field and potential as a result of the general shape of the sample, regardless the minor protrusions present in the sample's surface when treating the problem in an atomic scale; ii) the local variation of field and potential which results exactly from the atomic scale structure just mentioned. In this work we restrict ourselves in considering just the first case. We present an analytical solution of Laplace's equation in a region bounded by two surfaces held at constant but different potentials, i. e., in a region with boundary conditions such that we have a simple case of the Dirichlet problem /1/. We also discuss a few cases of practical interest, determining the ratio between field and potential at special points of the conductors. These special cases, are dispersed in the literature /2,3/, presenting sometimes conflict between them, and not always determined under the same approach as we do here.

For solving partial differential equations, the general methods available are the integral solution and the separated solution /2/. However, for a certain class of geometries, we can show that Laplace's solutions can be obtained from a much faster and straightforward method. We call it the single-valued Laplace's solution method and describe it as follows. For an orthogonal system of coordinates (q_1, q_2, q_3 and unit vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$) with metric coefficients h_1, h_2, h_3 (also known as scale factor /2/ and metric tensor since it is a second-rank tensor /4/), Laplace's equation can be written as:

$$\nabla^2 V = (1/H^3) \sum_{i=1}^3 (\partial/\partial q_i) [(H^3/h_i^2) (\partial V/\partial q_i)] = 0 \quad (1)$$

where V is the electric potential and

$$H^3 = h_1 h_2 h_3 \quad (2)$$

A coordinate surface for such a system corresponds to the loci of points where one of the coordinates is constant.

It can be shown /5/ that, for the set of orthogonal systems listed in Table 1, the solution of Laplace's equation in the region bounded by two coordinate surfaces, both related to the same coordinate, say q_1 , can be written as a function of just this coordinate. In a mathematical language this corresponds to state that, **if**

$$V = \alpha \text{ for } q_1 = a, \forall q_2 \text{ and } q_3; \quad (3.a)$$

$$V = \beta \text{ for } q_1 = b, \forall q_2 \text{ and } q_3 \quad (3.b)$$

with $\alpha \neq \beta$, and assuming also that it is possible to write

$$H^3/h_1^2 = h_2 h_3 / h_1 = f(q_1) g(q_2, q_3), \quad (4)$$

then the solution of Laplace's equation, V , depends only on q_1 and has the form

$$V = A \int [1/f(q_1)] dq_1 + B \quad (5)$$

where A and B are constants which are determined from the boundary conditions expressed by eqs. 3.

From the general expression for the gradient of V ,

$$\text{grad } V = (1/h_1) (\partial V/\partial q_1) \mathbf{e}_1 + (1/h_2) (\partial V/\partial q_2) \mathbf{e}_2 + (1/h_3) (\partial V/\partial q_3) \mathbf{e}_3, \quad (6)$$

it is possible to express the electric field at the region bounded by two coordinate surfaces (conditions 3, a and b) as:

$$\mathbf{E} = -A/[h_1 f(q_1)] \mathbf{e}_1 \quad (7)$$

The condition expressed by eq. 4 restricts the set of possible orthogonal systems for which a solution with the form of eq. 5 can be found and so the shape of the coordinate surfaces. In table 1 it is shown the possible geometries for coordinate surfaces of the various systems of coordinates we have considered.

Table 1 - Correspondence between coordinate surfaces and kind of geometry.

Coordinate systems	Coordinates	Coordinate Surfaces (corresponding number)*
Cartesian	$x \ y \ z$	1 1 1
Spherical	$r \ \theta \ \phi$	2 3 4
Circular cylinder	$\rho \ \phi \ z$	5 4 1
Elliptic cylinder	$\mu \ \phi \ z$	6 7 1
Parabolic cylinder	$\mu \ v \ z$	8 8 1
Parabolic (rotational)	$\lambda \ \mu \ \phi$	9 9 4
Paraboloidal	$\xi_1 \ \xi_2 \ \xi_3$	10 11 10
Oblate spheroidal	$\mu \ \theta \ \phi$	12 13 4
Prolate spheroidal	$\mu \ \theta \ \phi$	14 15 4
Conical	$\xi_1 \ \xi_2 \ \xi_3$	2 16 16
Ellipsoidal	$\xi_1 \ \xi_2 \ \xi_3$	17 18 19

* Each number above corresponds to a specific coordinate surface as listed below:

1. parallel planes; 2. concentric spheres; 3. circular cones of one sheet; 4. axial planes; 5. concentric cylinders; 6. confocal elliptic cylinders; 7. hyperbolic cylinders; 8. confocal parabolic cylinders; 9. paraboloids of revolution; 10. elliptic paraboloids; 11. hyperbolic paraboloids; 12. oblate spheroids; 13. hyperboloids of revolution (1 sheet); 14. prolate spheroids; 15. hyperboloids of revolution (2 sheets); 16. elliptic cones; 17. ellipsoids; 18. hyperboloids of 1 sheet; 19. hyperboloids of 2 sheets.

Table 2 - Expressions for electric field and potential for each kind of geometry of table 1 (bold-faced and non-italic letters).

Geometry	Potential	Field
parallel planes (1)	$V = A x + B$	$\mathbf{E} = -A \mathbf{e}_x$
concentric spheres (2)	$V = A / r + B$	$\mathbf{E} = A / r^2 \mathbf{e}_r$
cones of one sheet (3)	$V = A \ln \tan(\theta / 2) + B$	$\mathbf{E} = -A / [r \sin(\theta)] \mathbf{e}_\theta$
axial planes (4)	$V = A \phi + B$	$\mathbf{E} = -A / [r \sin(\theta)] \mathbf{e}_\phi$
concentric cylinders (5)	$V = A \ln(\rho) + B$	$\mathbf{E} = -A / \rho \mathbf{e}_\rho$
confocal elliptic cylinders (6)	$V = A \mu + B$	$\mathbf{E} = -A / [d (\cosh^2 \mu - \cos^2 \phi)^{1/2}] \mathbf{e}_\mu$
hyperbolic cylinders (7)	$V = A \phi + B$	$\mathbf{E} = -A / [d (\cosh^2 \mu - \cos^2 \phi)^{1/2}] \mathbf{e}_\phi$
confocal parabolic cylinders (8)	$V = A \mu + B$	$\mathbf{E} = -A / [2D (\mu^2 + \nu^2)^{1/2}] \mathbf{e}_\mu$
paraboloids of revolution (9)	$V = A \ln(\lambda) + B$	$\mathbf{E} = -A / [2D \lambda (\lambda^2 + \mu^2)^{1/2}] \mathbf{e}_\lambda$
elliptic paraboloids (10)	$V = A \ln (\xi_1^2 - a^2)^{1/2} + (\xi_1^2 - b^2)^{1/2} + B$	$\mathbf{E} = -A / [(\xi_1^2 - \xi_2^2)(\xi_1^2 - \xi_3^2)]^{1/2} \mathbf{e}_{\xi_1}$
hyperbolic paraboloids (11)	$V = A \ln (\xi_2^2 - a^2)^{1/2} + (\xi_2^2 - b^2)^{1/2} + B$	$\mathbf{E} = -A / [(\xi_2^2 - \xi_1^2)(\xi_2^2 - \xi_3^2)]^{1/2} \mathbf{e}_{\xi_2}$
oblate spheroids (12)	$V = A \tan^{-1} [\tanh(\mu / 2)] + B$	$\mathbf{E} = -A / [2d \cosh(\mu) [\cosh^2(\mu) - \cos^2(\theta)]^{1/2}] \mathbf{e}_\mu$
hyperboloids of revolution of 1 sheet (13)	$V = A \ln [1 + \tan(\theta / 2)] / [1 - \tan(\theta / 2)] + B$	$\mathbf{E} = -2A / [d \cos(\theta) [\cosh^2(\mu) - \cos^2(\theta)]^{1/2}] \mathbf{e}_\theta$
prolate spheroids (14)	$V = A \ln \tanh(\mu / 2) + B$	$\mathbf{E} = -A / [d \sinh(\mu) [\cosh^2(\mu) - \cos^2(\theta)]^{1/2}] \mathbf{e}_\mu$
hyperboloids of revolution of 2 sheets (15)	$V = A \ln \tan(\theta / 2) + B$	$\mathbf{E} = -A / [d \sin(\theta) [\cosh^2(\mu) - \cos^2(\theta)]^{1/2}] \mathbf{e}_\theta$
cones* (16)	elliptic integral	$\mathbf{E} = -A / [(\xi_1^2 - \xi_2^2)(\xi_1^2 - \xi_3^2)]^{1/2} \mathbf{e}_{\xi_2}$
ellipsoids (17)	elliptic integral	$\mathbf{E} = -A / [(\xi_1^2 - \xi_2^2)(\xi_1^2 - \xi_3^2)]^{1/2} \mathbf{e}_{\xi_1}$
hyperboloids of 1 sheet* (18)	elliptic integral	$\mathbf{E} = -A / [(\xi_2^2 - \xi_1^2)(\xi_2^2 - \xi_3^2)]^{1/2} \mathbf{e}_{\xi_2}$
hyperboloids of 2 sheets* (19)	elliptic integral	$\mathbf{E} = -A / [(\xi_3^2 - \xi_1^2)(\xi_3^2 - \xi_2^2)]^{1/2} \mathbf{e}_{\xi_3}$

*elliptic

2. CASES OF PRACTICAL INTEREST

From a total of thirty three coordinates in table 1, only nineteen correspond to distinct geometries. From these, four cases do not present an analytical solution since it would be necessary to solve elliptical integrals. The other fifteen have an analytical solution and Table 2 presents the general form of the expressions for the electric potential and field.

From the fifteen cases above mentioned, six can be considered as being of practical interest: concentric spheres, circular cones (one sheet), concentric cylinders, paraboloids of revolution, prolate spheroids and hyperboloids of revolution (2 sheets). Frequently, for emitters or other sharpened conductors, it is possible to measure the electric potential with great accuracy (0.01% or even less) but the field determination

depends on geometric characteristics of the sample which are expressed by the field proportionality factor, i. e., the ratio between field (F_0) and potential (V_0) at close vicinity of the apex of a conductor with sharp geometry. It is then expressed by

$$\beta = F_0/V_0 \quad (8)$$

Several authors have determined the value of β for various geometries /6 - 10/, with or without approximations, getting sometimes slightly different results as a consequence of the referential for the electric potential. We present values of β for a few cases of interest in table 3.

Table 3 - Field proportionality factor for some geometries of practical interest ($\beta = F_0/V_0$)

geometry	β (exact)	β (approximation)
spherical	$1/r_t$	-
concentric cylinders	$1/[r_0 \ln(R/r_0)]$	-
hyperboloid	$4d/[[-r_t^2 \pm r_t(r_t^2 + 4d^2)^{1/2}][\ln ((2d + (r_t^2 + 4d^2)^{1/2})/r_t)^{\pm 1}]]$	$1/[r_t \ln(2(d/r_t)^{1/2})]$
paraboloid	$2/[r_t \ln(2D/r_t)]$	-
prolate spheroid	$4d/[[r_t^2 \pm r_t(r_t^2 + 4d^2)^{1/2}][\ln ((2d + (r_t^2 + 4d^2)^{1/2})/r_t)^{\pm 1}]]$	$1/[r_t \ln(2(d/r_t)^{1/2})]$
conical	diverges	diverges

r_t = radius of curvature;

R = external radius of the cylinder;

d = focal distance (ellipse/hyperbola);

D = constant

r_0 = internal radius of the cylinder

3. FINAL COMMENTS

We have determined the expressions for the field and electric potential in several regions where it is possible to solve Laplace's equation by adopting as boundary conditions a constant potential at each one of two different coordinate surfaces. This has been done using a general theorem where the basic requirement is that expressed by eq. 4. The ratio between field and potential at the vicinity of the apex of a few sharpened geometries was then calculated.

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