Field enhancement factor: A self-validating method

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A general method is presented for calculating the field enhancement factor of cylindrically symmetric high aspect ratio conductive structures. A discrete distribution of charges is used on the symmetry axis to replace the real charge distribution such that the electrostatic potential satisfies a set of boundary conditions. Their number will be set through a self-validating process. The method is exemplified for the geometric structure of a carbon nanotube and a conical tip, while the advantages are weighted against commonly used theoretical models.

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While practically very important, the computation of the static electric potential distribution around an electrically conductive high aspect ratio feature has been a challenging analytical, as well as numerical, problem. The electron field emission process is an outstanding example where the accurate description of the electric potential distribution surrounding the emitting tip is essential. The importance of this problem extends also over a broad range of other practical applications where it is becoming increasingly more difficult to solve it for various geometries of conductive high aspect ratio structures (CHARS). The preferred general route used in many of the cases is to employ a numerical simulation software package that is able to reproduce a given structure and obtain the electric field in a desired point. However, there are a number of limitations for simulation packages, such as insufficient work space points and the roughness of the mesh unit around a sharp protrusion, which combined with the lack of direct experimental evidence for comparison, makes it impossible to validate a particular solution.

The present paper aims at suggesting a general procedure to compute the electric potential distribution surrounding a cylindrically symmetric CHARS, using a self-validating procedure. This method is based on the following numerical principle: consider the Laplace equation in a certain empty region of space. If the values of the potential are specified with high accuracy on a certain area of the boundary, close to some point of it (for example the origin of the space), but is otherwise loosely defined in other remote points on the boundary, then a family of solutions for the potential are generated which converge to each other in the close neighbourhood of this origin. In other words, by specifying accurately the values of the potential close to some given point, the solution of the Laplace equation will be accurate near this point, regardless of the remote boundary conditions. For the particular case of a CHARS placed in an electric field, the region of interest is obviously near the tip. Therefore, by specifying with enough accuracy the potential on the tip, one may expect that the solution of the Laplace equation is also correct in its close neighbourhood. Following this principle, we propose to replace the real charge distribution on the CHARS’s surface with a system of virtual charges such that the total potential satisfies strict boundary conditions on a limited area of the tip. For simplicity, we consider the conductive feature as grounded. The obtained spatial distribution of the potential in the region close to this surface is thus self-validating
since the system of charges can be modified in order to minimise the distance between the zero-voltage equipotential and the real grounded conductive surface in the vicinity of the tip. Once the optimum potential distribution is obtained, the local electric field can be calculated in a given point. The most targeted applications are the CHARSs, where advantage can be taken of the electrostatic property of field enhancement. If the cathode is considered to be surrounded by a uniform electric field $F_0$ (usually called the applied or macroscopic electric field), then, according to Gomer [1], the field enhancement factor for a CHARS (commonly denoted in the literature as $\beta$) can be defined as the ratio between the strength of the local electric field at its tip and the value of $F_0$. The computation of $\beta$ will be exemplified for two particularly interesting shapes of CHARS: conical and cylindrical.

Let us thus consider first a cylindrically symmetric conductive conical surface of base angle $\alpha$, terminated smoothly by a spherical sector of radius $r_0$, as shown in Figure 1. The height $H$ is measured from its base to the tip and its aspect ratio is defined as $\Delta = H r_0^{-1}$. The base radius can be expressed as: $a = H \cos \alpha \sin^{-1} \alpha + r_0 (1 - \cos \alpha) \sin^{-1} \alpha$. The structure is considered to be mounted on an infinite grounded $(xOy)$ conductive plane such that its surface is a $0$ V equipotential. Following the method described above, the charge distribution on the surface of the structure will be replaced by a system of $N+1$ virtual co-axially charged rings of radii $r_i(\alpha)$ and charges $q_i(\alpha), i = 1, N+1$, such that the distance from any ring to the real surface is $r_0$. The rings are equidistant to each other, such that their positions from the base of the cone are given by $z_i = i(H - r_0)/N, i = 1, N$ and the $N^{th}$ ring reduces to a point placed in the centre of the spherical sector. The $N+1$ ring is also a point charge $(r_{N+1}(\alpha) = 0)$ placed at $z_{N+1} = H - r_0 + d$. The radius of each charged ring is given by: $r_i(\alpha) = a - r_0 \sin^{-1} \alpha - i d \cot \alpha, i = 1, N$. In order to be equivalent to the original structure, the system of charged rings and the externally applied field must produce a vanishing potential on the surface of the replaced structure. Obviously, such a strong condition cannot be fulfilled by a simple set of equivalent charges. Instead, the total potential of the virtual charges must cancel in a discrete set of points on the surface of the original structure. Moreover, as the main interest in at CHARS electric behaviour is normally in its tip region, the obtained 0 V equipotential should map as accurately as possible the physical surface of the structure. Therefore the problem to be solved is as follows: find the number of charged rings and their
individual magnitudes such that the 0 V equipotential of this system best matches the surface of the structure in the tip region.

The normalized potential of an individual ring and its image in the grounded infinite plane at the base of the cone at some exterior point, \((r, z)\), is given by:

\[
\eta_1(\alpha) = \int_0^{z \alpha} \left( \frac{\lambda(\alpha)}{\sqrt{(\zeta - \zeta_0)^2 + \rho^2 + \rho^2 - 2\rho \rho \cos \varphi}} - \frac{\lambda(\alpha)}{\sqrt{(\zeta + \zeta_0)^2 + \rho^2 + \rho^2 - 2\rho \rho \cos \varphi}} \right) \, d\varphi.
\]  

(1)

The total electrostatic potential of the \(N+1\) charges can be readily expressed as:

\[
\eta(\rho, \zeta) = -\zeta + \sum_{i=1}^{N+1} \eta_i(\alpha),
\]

where the variables have been normalized to the tip radius \(r_0\):

\[
\eta(\rho, \zeta) = V(\rho, \zeta)(F_0 r_0^{-1}), \quad \lambda_i(\alpha) = q_i(\alpha) \left( 8\pi^2 \varepsilon_0 F_0 r_0^2 \right)^{-1}, \quad \zeta = z r_i^{-1}, \quad \zeta_0 = z_i r_0^{-1}, \quad \rho = r r_0^{-1}
\]

and \(r_i = r_i r_0^{-1}\). The notation \(\delta = d r_0^{-1}\) will also be useful. The unknowns in Eq. (1) are the normalized charges \(\lambda_i, i = 1, N+1\) and can be found if the following boundary conditions are simultaneously satisfied:

\[
\eta(\rho_j^c, \zeta_j^c) = 0, \text{ for } j = 1, N+1,
\]  

(2)

where, \(\rho_j^c = a r_0^{-1} - \sin^{-1} \alpha + \sin \alpha - j(\Delta-1)N^{-1} \cot \alpha, \quad \zeta_j^c = \cos \alpha + j(\Delta-1)N^{-1}, j = 1, N, \quad \rho_{N+1}^c = 0 \) and \(\zeta_{N+1}^c = \Delta\) are the radii and vertical positions of the circular boundary conditions imposed on the real conical surface. From the depiction in Figure 1 it can be seen that the distance from a point on a charged ring (shown in red) to a circular boundary condition line directly above (shown in blue) is exactly the tip radius. The number of equations in the system defined by Eq. (2) will vary depending on the number of charged rings placed on the axis, thus numerical computation was used to solve it. The number of charges is the key parameter in this model and will be obtained from the self-validating method which will be detailed below.

The solution of Eqs. (2) allows for the calculation of equipotential profile surfaces given by the coordinate pair \((r, z)\). In the ideal case, the 0 V equipotential should be the surface of the structure. We propose to use the distance between the obtained 0 V equipotential and the spherical sector at the tip as a measure of the accuracy of approximating the real potential in
this region by the superposition of the potential of the external field and the considered system of point charges. Therefore, if \( z_0(r) \) and \( z_{\text{cap}}(r) \) are the cross-sectional profiles of the 0 V equipotential and the cap of the structure, then the following quantity can be required to be at a minimum:

\[
\epsilon_e = \frac{1}{r_0} \max_{0 \leq \rho \leq r_0} \left| z_0(r) - z_{\text{cap}}(r) \right|
\]  

Minimising Eq. (3) with respect to the two model parameters, \( N \) and \( d \) leads to the best configuration of the 0 V equipotential in the cap region closest to the potential of the real configuration. Then, the electric field can be obtained from the \( z \)-component of the gradient of the potential. The enhancement factor will be given by the ratio between the electric field at the tip, calculated for \( \rho = 0 \) and \( \zeta = \Delta \), and the uniform macroscopic electric field, \( F_0 \):

\[
\beta(\alpha) = 1 + 2\pi \sum_{i=1}^{N-1} \lambda_i(\alpha) \left[ \frac{\Delta - \zeta_i}{\sqrt{(\Delta - \zeta_i)^2 + \rho_i^2}} - \frac{\Delta + \zeta_i}{\sqrt{(\Delta + \zeta_i)^2 + \rho_i^2}} \right]
\]

Using the described method, it is therefore possible to obtain the electrostatic potential and ultimately the enhancement factor for a conical CHARS terminated smoothly by a spherical sector, as a function of the base angle \( \alpha \). It can be readily observed that the generality of this method includes the case of a capped cylinder (ex. A conductive carbon nanotube) when \( \alpha = 90^\circ \). The charged rings will be then transformed into point charges positioned on the symmetry axis, while the radii of the circular boundary condition lines are equal to the radius of the tip \( r_0 \). Figure 2 shows calculated equipotential lines surrounding a conical and a cylindrical CHARS of equal height and aspect ratio. In order to obtain the 0 V equipotential (shown in blue), we have split the normalized interval \( \left( 0, \alpha_0^{-1} \right) \) in a fine grid and searched for the values of \( \zeta \) such that \( \eta(\rho, \zeta) = 0 \) for the number of charges that minimizes Eq. (3) in the tip region. The obtained surface is not that of a perfect hemisphere. However, according to the self-validation condition in Eq. (3) it is the best approximation spherical sector at the tip. Typical values for the minimum of \( \epsilon_e \) is of the order of \( 10^{-3} \). The next three lines shown in light blue, orange and red are the calculated equipotentials for 0.5, 1 and 1.5 V, respectively. After obtaining the best approximation for the potential profiles, Eq.
can then be used to find the value of the enhancement factor. At this point it is important to outline the differences between the presented method for calculating the field enhancement factor and existing methods in the literature.

The specialised articles on the subject of field enhancement factor can be roughly divided into three methods: the direct analytical approaches, the numerical approaches and image-charge-type methods. The purpose of each of the three approaches is to obtain a simple and functional relationship between the enhancement factor and the geometrical parameters of the system. Forbes et al. published a comprehensive review of the most popular results obtained for the field enhancement factor [2]. Analysing the various formulas obtained by different groups (and several variations found in the literature [3-13]) it appears that there is hardly any correlation between the results obtained from the various approaches, which poses the obvious question as to which method should be used with a real system. It has thus become evident that the crucial step of comparing the electrostatic potential profile obtained through a particular method with the surface of the studied system in the region of interest was missing from all but the Dyke et al. [3] works. However the formula which they proposed is restricted to conical structures terminated non-smoothly by a spherical sector. The method proposed in this paper allows the computation of the enhancement factor through such a self-validation procedure as a function of the aspect ratio and the base angle of a conical CHARS. For \( \alpha = 90^\circ \), the case of a capped cylinder is obtained and the dependence on its aspect ratio can be calculated. Figure 3 shows the dependence of the enhancement factor on the base angle of the structure for five values of the aspect ratio, 50, 70, 100, 150 and 200. As it can be seen the enhancement factor has a strong dependence on both the aspect ratio and the base angle, which suggests that a simple unifying formula may not be available. Obviously, for the case of a capped cylinder, there is no base angle dependence and the model is confirming the general hypothesis in the literature that the enhancement factor is only dependent on the aspect ratio. A linear fit of the five points can be used to obtain a simple formula to quickly estimate the enhancement factor for aspect ratios between 50 and 200.

\[
\beta_{\text{approx}} (\Delta) = 10.63 + 0.62 \Delta, \quad (5)
\]

However, we must point out that outside this range, especially at small values of \( \Delta \), the constants in Eq. (5) have to be recalculated. Indeed, the text-book example of the hemisphere
on a plane (Δ=1) in a uniform electric field [14] the enhancement factor is 3, which is obviously different from the corresponding result of Eq. (5). This limiting case is useful for outlining the role of the other model parameter (besides N), namely the position d of the N+1 charge with respect to the centre of the hemisphere. For the case of the hemisphere-on-a-plane problem (α = 90° and H = r₀) there is only one charge needed, which is placed at a distance d from the centre of the hemisphere. If the parameter d is chosen such that \( d^2 \frac{\epsilon}{\epsilon_0} \leq 1 \) then, according to Eq. (4), \( \beta \geq 3 \). It follows that, for structures with low aspect ratios it is more likely that the parameter d plays a more important role and that the optimisation of \( \epsilon \) in such cases has to be performed effectively with both model variables.

In conclusion, we have constructed a general field enhancement model applicable to cylindrically symmetrical conductive structures using a sequence of virtual charges which create the electrostatic equivalent of the original system if suitable boundary conditions are imposed to the electrostatic potential. A self-validating condition was added to this model in order to optimize the accuracy of the calculated potential. This model was shown to be applicable to capped conical as well as cylindrical structures placed in a uniform electric field. The distance between the 0 V equipotential obtained from the proposed model and the grounded surface of the given geometry was minimized in order to obtain the optimum number of charges. Using this model, we have obtained the equipotential lines with good accuracy, as well as the dependence of the enhancement factor on the base angle of the conical CHARS for several values of the aspect ratio. Using a linear fit, a simple formula was found for the limiting case of the cylinder (the base angle \( \alpha = 90° \)) that can be readily used in practical situations.
References:


Figure captions:

Figure 1: Sketch of the conical structure terminated smoothly by a spherical sector of radius $r_0$ and the system of charged rings (shown in red). Represented in blue are the locations where the boundary conditions are imposed in Eq. (2) (drawing not to scale!).

Figure 2: Equipotential profiles around smoothly caped conical ($\alpha = 75^\circ$) and cylindrical ($\alpha = 90^\circ$) structures calculated using the self-validating model. The blue points represent elements of the constructed 0 V profile while the light blue, orange and red lines are calculated profiles for the 0.5, 1 and 1.5 V
equipotentials, respectively. The geometrical dimensions have been normalized with respect to the tip radius for visual purposes.

Figure 3: Dependence of the enhancement factor as a function of the base angle of the structure for different values of the aspect ratio. The enhancement factor increases as the structure approaches the shape of a cylinder. This case is shown as hollow symbols.
Figure 1

Figure 2
Figure 3