Estimation of the area of field emission of a carbon nanotube using modelling in COMSOL Multiphysics

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Abstract. In this paper, the computer simulation methods were used to study the effect of the mutual shielding in the multi-point system of a nanoscale field cathode on its current-voltage characteristics and the characteristic parameter of the field emission area. Modeling is carried out in the COMSOL Multiphysics software package. Geometric parameters of the model correspond to the parameters of carbon nanotubes. As a result of the simulation, the dependence on the distance between the emission centers of the shape of the current-voltage characteristic of the central emitter, the effective current density of the entire emission system, and the size of the field emission area were constructed.

1. Introduction
Field emitters are complex systems for analyzing their properties and characteristics. The process of field emission depends on many external and internal factors. Computer modeling is one of the effective methods for studying such complex systems, while analytical studies are difficult. The emission characteristics of field emitters are affected by the distribution of the field enhancement factor β, which in turn depends on the geometry of the emission system, namely, the shape, aspect ratio and radius of the rounding of the emitter vertices, and the magnitude of the interelectrode gap.

The decrease in the distance between nanoscale emitters increases their number, which can be located at a given area of the cathode, and accordingly the total emission current, but at the same time, the mutual screening effect reduces the fields on their surface and accordingly the total current falls. Thus, it is obvious that there is an optimal distance between the emitters, which makes it possible to achieve the maximum emission current from the cathode of a given area.

The paper [1] presented a three-dimensional model for estimating the electrostatic properties of a single-point field emitter characterized by the geometry of the hemisphere on the cylinder. Numerical simulation was performed by the finite element method using the Ansys-Maxwell software. As a result, the distribution of the electric field on the surface and near the emitter was obtained. The modeling and analytical calculation correlated well with each other. The dependences of the β on the aspect ratio of the emitter and on the ratio of the interelectrode distance to the emitter height were obtained. In work [2] a simulation of electrostatic fields in COMSOL Multiphysics has been created to predict the field enhancement factor β of real emitters with different tip radii. In article [3], the effect of mutual screening of emitters consisting of an array of carbon nanotubes (CNTs) was investigated using 3D modeling in SIMION 8.0 software and its effect on the efficiency of electron emission was
demonstrated. The simulated case of nine CNTs arranged in three rows of three columns showed that the local electric field of the central CNT is lower than one of its neighbors, but less than one of an isolated nanotube. The analytical dependence of the field enhancement factor β on the distance between the emitters in triangular and quadrangular arrays was calculated in [4] using the LCM (Line Charge Model) method. With the help of the dependence obtained, the dependences of the current density on the value of the external electric field were calculated. The obtained dependences have peaks on which the optimum distances between the emitters corresponds to the maximum currents was determined. Similar calculations were conducted in article [5]. The effect of screening at the edges of the arrays of tips with the help of analytical modeling by the LCM method was investigated in article [6]. The authors showed that a decrease in the distance between the external and adjacent emitter of the array increases the screening and, consequently, decreases the field enhancement factor of the emitters near the edge of the array.

In this paper we modeled the distribution of the electrostatic field in a symmetric system of multi-point field cathode consisting of several CNTs and carried out a study of the influence of the mutual screening effect on the current-voltage characteristic (IVC) and the field emission area.

2. Modeling of the emission system

The software package COMSOL Multiphysics solves the Laplace equation by the finite element method and extracts values of the electric field at any point of the surface and volume of the investigated model. The system of a multi-point field cathode consists of the nine tips (CNTs) which have a form of cylinders with hemispheres on the vertices. The parameters of the tips in our model are the same: radius \( r = 0.5 \, \text{nm} \) and height \( h = 500 \, \text{nm} \). Tips are located on the "cathode" plane below the "anode" plane (distance between the planes \( D_{\text{an-c}} \) was set 2 \( \mu \text{m} \)). The Dirichlet boundary condition was specified at the electrodes surfaces: a ground state for "anode" and a positive potential (applied voltage \( U \)) for "cathode". To avoid the edge effect, we applied the Neumann boundary condition, so the potential distribution at the edges of the model region (total cylinder where all electrodes were located) has linear changes only in the direction of the Z axis. The distance between central and peripheral emitters \( d \) was varied from \( 0.05h \) to \( 5h \). The selected voltage range produces an acceptable level of the electrostatic field at the tips vertices (up to \( 1.5 \times 10^{10} \, \text{V/m} \)) and level of the current which is appropriate for nanotubes (registered and non-destructive).

After the settings of the basic parameters of model in COMSOL the module "electrostatics" automatically selected the morphology and density of the mesh (Fig. 1a). The regions around tips are critical and require the high density of the mesh, therefore we set a triangular grid with side dimensions equal to \( 5 \times 10^{-10} \, \text{m} \) at the surface of tips vertices (Fig. 1b). For the anode and cathode planes the triangular grid was constructed with the minimum and maximum dimensions of the triangles sides \( 7.2 \times 10^{-8} \) and \( 4 \times 10^{-7} \, \text{m} \), respectively.

As a result of the modeling the potential distribution in the space and on the surface of the system (Fig. 1c) and the contour lines of the electric field distribution (Fig. 1d) were obtained. The maximum value of the electric field was \( E_{\text{max}} = 8.6 \times 10^{9} \, \text{V/m} \) at a radial distance between the central and peripheral emitters \( d = 0.05h \). It is clear that distortion of the electric field contour lines caused by the screening effect of the tips. The field distributions on the cathode surface was modeled for the applied voltage range \( 17.5 \div 55 \, \text{V} \) at different radial distances \( d \).

3. Calculation of the current density and emission area

To calculate an emission current density \( j \), which depends on the local electric field \( E \), we used the Elinson [7] analytical formula:

\[
j = A_{\varphi}(E)^2 \cdot 10^{\frac{B_{\varphi}}{E}}.
\]

where \( A_{\varphi} \) and \( B_{\varphi} \) are functions that depend on the work function of the material. The work function value we took from [8, 9] for CNT: \( \varphi = 4.6 \, \text{eV} \).
Figure 1. The COMSOL model at $U = 55$ V: calculating meshes of the all model (a) and of one of the tips (b), distribution of the electric potential (c) and of the electric field (d), the distribution of the current density on the surface of central (e) and peripheral (f) tips.

The calculated current density distribution on the surface of the central and outside tips are presented at Fig. 1e,f. The distribution of the outside tip is displaced from the center of the vertex due to influence of the neighboring tips.

To investigate the mutual screening effect of the tips we varied the distance $d$ in the range from $5h$ to $0.05h$ and calculated total current dependence on voltage of the central tip. The corresponding IVCs are presented at Fig. 2a. It is obvious that the IVCs, starting with a distance equal to $5h$ weakly depends on the distance since it has become too large and the tip fields affect each other in a less degree. When the distance $d$ is increasing the compression of the IVC to the abscissa axis is observed as a consequence of the increase of mutual screening on the tips. At $d = 0.05h$ the emission current is of the order of $1$ pA.
Current-voltage characteristics were calculated by integrating the current density of an array of emission objects by COMSOL. As noted earlier, on the one hand, the magnitude of the emission current depends on the number of emitters per unit of surface, but on the other hand the increasing effect of their mutual screening reduces the fields on their surface that entails a total current drop.

The effective current density $J_{\text{eff}}$ of the all system:

$$J_{\text{eff}}(U, d) = \frac{I_z}{\pi d^2},$$

where $I_z$ is the total current of the whole array of emitters; $d$ is the radial distance between the central and peripheral tips.

To estimate an optimal ratio of radial distance to height of the tips $d/h$ we calculated an effective current density $J_{\text{eff}}$ at different voltages (Fig. 3a). From the constructed dependences it follows that each curve in the family has a maximum at the corresponding ratio $d/h$. These maxima were shifted to the left with increasing in the applied voltage: from 1.1 to 0.7. Fig. 3b shows this shifting of the maximum for the minimum and maximum applied voltages (37.5 V and 55 V).

The calculation of the field emission area was made in two ways. The first way is analytical. It requires calculation of the current density at the top of the emitter, an experimental measurement of which cannot be performed [10, 11]. Corresponding area $S_c$ (so called "notional area") is:

$$S_c = \frac{I}{f_{\text{max}}}$$

Figure 2. Calculated IVCs (a) and IVC-FNs (b) of the central tip for different inter-tip distances.

Figure 3. Dependence of the calculated effective current density $J_{\text{eff}}$ of all emitter array on the ratio $d/h$ for different applied voltages (a) and for minimum and maximum applied voltages (b).
where \( j_{\text{max}} \) – the maximum density of the emission current calculated by formula (1), \( I \) – the current computed by integrating \( j \) over the surface of the CNT (rounded end face of the model emitter) by means of COMSOL.

The obtained family of dependencies \( S_c \) on the applied voltage \( U \) at the different distances \( d \) are presented at Fig. 4a. As can be seen, the value of \( S_c \) nonlinear decreases with the decreasing in inter tip distance \( d \) at a fixed voltage.

The second way is experimental, since it uses the values of the experimental IVCs. It requires calculation of the effective slope \( b \) and intercept \( a \) of the IVC in the Fowler-Nordheim coordinates (IVC-FN), which can be obtained using approximation of the IVC-FN by a straight line. Corresponding effective area \( S_{\text{eff}} \) [9] is:

\[
S_{\text{eff}} = \frac{10aR^2}{\Lambda_\phi R^2}
\]

(4)

Note that \( S_{\text{eff}} \) is an integral characteristic, averaging the IVC over the entire voltage range.

To estimate the effective field emission area \( S_{\text{eff}} \) and its dependence on the voltage, we translated the IVCs of the central tip into the Fowler-Nordheim coordinates (Fig. 2b) and estimated cutoffs of the corresponding trend lines.

The effective field emission area dependence on the inter tip distance \( d \) is presented at Fig. 4b. The emission area increased to 1 nm². It is 63% of the total area of the hemisphere vertex which is equal to 1.57 nm². Comparison of the emission areas \( S_c \) and \( S_{\text{eff}} \) has shown that the effective area exceeds the conditional area over the entire voltage range and for all values of \( d/h \). The ratio \( S_{\text{eff}}/S_c \) for \( d/h = 0.6 \) with the increase in voltage varies from 4.9 to 1.9, and for \( d/h = 5 \) from 3.7 to 1.5.

![Figure 4](image)

Figure 4. Calculated field emission areas of the central tip for variance of the ratio \( d/h \) from 0.6 to 5: the notional area \( S_c \) depending on the applied voltage (a) and the effective area \( S_{\text{eff}} \) averaging the IVC over the entire voltage range (b).

4. Conclusion

The distribution of the electric fields on the surface of a nanostructured multi-point field cathode consisting of the nine parallel conducting tips was modeled in COMSOL Multiphysics. By post-processing of the simulation results the distribution of the emission current density over the emitter surface was obtained and corresponding IVCs were constructed.

To estimate an optimal inter-tip distances \( d \) when effective current density \( j_{\text{eff}} \) is maximal we calculated \( J_{\text{eff}} \) at different voltages in range 37.5 to 55 V. It is established that these maxima are subject to displacement to the left with increasing applied voltage. The obtained results confirm the similar calculations made in the works of leading foreign scientists in the branch of field emission [4-5].

The change in the value of the optimum distance between the emitters with increasing voltage level is associated with a change in the relative contribution of each CNT to the total I-V characteristic. This change is reflected in the IVC-FN form, making it different from the straight line. This curvature can
be seen on the plot of the effective area versus the voltage Fig. 4b, which is determined by cutting off the trend line.

To estimate the effective emission area $S_{eff}$, the IVCs of the central tip were translated into the FN coordinates. It’s clearly seen, that emission area increased to 1 nm², what is 63% of the total area of the vertex of the tip, equal to 1.57 nm².

The dependence of the notional field emission area $S_0$ of the central tip on the applied voltage was obtained. From the obtained family of dependences, it is shown there is a nonlinear decrease with the decreasing in the inter tip distance $d$ at a fixed voltage.

It is worth noting that the presented solution for field distribution is valid for any system with appropriate scaling, especially for carbon nanotubes. But the shielding effect most important for multi-tip nanoscaled field emission systems with distributed current load. Our results are of interest for investigations of field emission systems with a dense arrangement of CNTs [12]. Such systems are widely used in field emitters, which consist of ordered CNT and tips arrays [13-14].

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