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Simulation of nanocomposite field emitters in COMSOL Multiphysics using field emission projector data

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Abstract. The aim of this work is simulation of the surface of multi-tip field emitters in the COMSOL Multiphysics package using experimental data processing. The data of the spatial arrangement of the emission sites and their sizes were obtained by processing the glow patterns of the field emission projector and macroscopic volt-ampere characteristics in the LabView software package. The experiment was carried out for a nanocomposite field emitter based on a multiwall carbon nanotubes and a polymer. As a result, a surface model was constructed. It allows to carry out a variety of virtual studies that are necessary for deeper understanding of the effects and processes occurring in the multi-tip field emission systems.

1. Introduction

The multi-tip field emitters based on carbon nanotubes (CNTs) has many applications. They are basis for the production of flat displays, cathode ray tubes, planar light sources, microwave amplifiers and portable X-ray machines, serve as electron sources for high-resolution electron microscopy, electron beam deposition, electron beam lithography etc. [1].

Field emitters are complex systems for analyzing their properties and characteristics, since the field emission process depends on many external and internal factors. Methods of mathematical modeling allow to identify the main factors that determine emission properties, to predict the evolution of characteristics, to study the response of a simulated physical system to changes in its parameters and initial conditions.

One of the factors influencing the emission properties is the relative position of the emission sites in a dense array. The intensity of the surface electric field and, consequently, the field enhancement factor (FEF) of each emission site in array is less, than if it would have been isolated. This phenomenon is known as the mutual screening effect [2].

It was shown in [3] that in order to achieve a complete absence of the screening effect in the CNT based field emitters, the nanotube should be placed at a distance equal to their own fivefold height. An experiment performed in [4] clearly demonstrates this effect.

According to the article [5] the FEF at the vertices of CNTs increases due to their location in elevated areas – the microscopic roughness of the field cathode surface. In addition, it was analytically shown that on the top of nanotubes located on the protrusions the multiplication operation acts: the FEF of vertices of microscopic protrusions without nanotubes is multiplied by FEF of this nanotubes located on a flat conducting substrate without protrusions.
Non-oriented nanocomposite structures based on CNTs are one of the most promising materials for the production of field cathodes (cheap in fabrication, least susceptible to destructive processes in a technical vacuum, demonstrate high emission currents). A nanocomposite large-area field emitters (LAFE) that we used in our experiments belong to the specified type. They consist of a polystyrene matrix and a filler, which is an unordered multi-layered CNTs. This type of emitters has a very complex morphology: the polystyrene matrix forms a hilly surface and the CNTs protruding above it are oriented randomly and in places form bundles (Fig. 1). Due to this microscopic roughness a significant amplification of the electric field is achieved.

In the presented work, we constructed a model of a multi-tip field emitter based on single wall carbon nanotubes in polystyrene (SWCNT/P). Modeling was provided in the COMSOL Multiphysics software package on the basis of experimental data obtained as a result of processing the glow patterns of a field emission projector. Data on the spatial arrangement of the emission sites and their geometric parameters were obtained from the glow patterns and current-voltage characteristics (IVC) using algorithms implemented in the software package LabView [6].

2. Getting the source data about the simulation object
An accurate virtual reproduction of the nanocomposite emitter surface (Fig. 1a) is impossible today. To avoid this problem we have presented each emission site in the form of a hemisphere (microscopic roughness) and a vertical cylinder with a rounded vertex (with dimensions, coinciding with the passport data of the experimental CNTs) located at the top of the hemisphere (Fig 1b).

![Figure 1](image1.png)

Figure 1. Scanning electron microscope photograph of the surface area of a sample of LAFE, at which potential emission sites are present - microscopic protrusions of nanocomposite with protruding ends of CNTs on it (a). Structural unit of the simulated nanocomposite emitter (SWCNT/P), which is a model of a CNT in the form of a rounded cylinder, located on a hemisphere imitating for it an elevation (b).

Figure 2 shows the scheme for constructing of the effective surface of nanocomposite LAFE. Firstly, the process of identifying individual positions of emission sites at a given current level is initiated. The location of the emission sites corresponds to bright peaks in the glow pattern (Fig. 3). To separate the brightness peaks of emission sites from the digital noise of the USB video camera, the line filter IMAQ Convolute VI is used.

In Figure 3, the detected brightness maxima are presented in the form of white dots, which correspond to individual emission sites. The glow pattern continuously changes due to adsorption-desorption processes on the emitter surface. Therefore, in order to register each emission site, we continuously sum up the black and white images until the total area of the white zones in the total image reaches saturation. This process takes several minutes while maintaining a constant level of current $I_0$. The detailed description of the technique for processing of glow patterns is presented in [6, 7].
As a result of the recognition of the glow pattern (Fig. 3) at a current level of ~ 1.5 mA, we have the coordinates of each detected emission site (Fig. 4).

![Figure 2](image2.png)

**Figure 2.** General scheme of the sequence of operations for constructing a surface model of nanocomposite LAFE.

![Figure 3](image3.png)

**Figure 3.** Glow pattern, corresponding to the locations of the emission sites.

![Figure 4](image4.png)

**Figure 4.** The coordinates of the emission sites obtained by the field emission projector.

We assumed that the brightness level of each emission site $Y_{es}$ in the glow pattern is proportional to the corresponding local emission current $I_{loc}$ at each instant of time. Consequently, the current loads of the emission sites can be calculated from the total macroscopic current $I$ measured using the IVC recording and processing module, using the maximum brightness of the emission sites $Y_{es}$ in the form of weighting coefficients

$$I_{loc} = Y_{es}C = Y_{es} \frac{I}{\sum Y_{es}}$$

(1)

where $C$ is the coefficient of proportionality, $Y_{es} = \max(Y_{es})$ - the maximum brightness of the emission site, registered for the whole period of accumulation. Thus, the resulting histograms represent the emission activity of all registered emission sites without the influence of adsorbates.
Corresponding to the distribution of the maxima local currents, the distribution of the effective field enhancement factors $\beta_{\text{eff}}$ (Fig. 5) is obtained by solving the Fowler-Nordheim equation in the Elinson-Shrednik approximation with respect to the FEF [8]:

$$I_{\text{loc}} = A_{\text{eff}} A_\varphi (E_M^\beta_{\text{eff}})^2 \cdot 10^{E_M^\beta_{\text{eff}} / B_\varphi}$$

(2)

$$A_\varphi = \frac{1.4 \cdot 10^4 \sqrt{\varphi}}{\varphi}$$

(3)

$$B_\varphi = -2.82 \cdot 10^7 \varphi^{3/2}$$

(4)

where $A_\varphi = 3.39014 \cdot 10^{-5}$ and $B_\varphi = -2.78218 \cdot 10^{8}$ – coefficients calculated for the work function of CNTs $\varphi = 4.6$ eV [9]. $E_M$ – a macroscopic field calculated as the ratio of the voltage to the interelectrode distance $U/d$, $A_{\text{eff}}$ – the effective area of the CNT emission, which we assumed to be $1.8 \, \text{nm}^2$ [10].

To translate the experimental distribution of $\beta_{\text{eff}}$ reached at the top of the CNTs of a real sample to the radii of the hemispheres $R$ on which they are located, the FEF dependence at the top of the CNT $\beta_{\text{max}}$ on the radius of the hemisphere $R$ in COMSOL was simulated. The parameters of the model were set to the same as in the experiment: the radius of the CNTs $r = 1 \, \text{nm}$ and the interelectrode distance $d = 300 \, \mu\text{m}$, the height of the CNTs was assumed to be the same and equal to $2.5 \, \mu\text{m}$ (this value was chosen to bring the model FEFs into the experimental FEF range).

**Figure 5.** The distribution of the field enhancement factor $\beta$ over the surface of the model nanotube with maxima value

**Figure 6.** The distribution of radii of hemispheres $R$ obtained by substitution of experimental $\beta_{\text{loc}}$ in approximated dependence. In the inset: a curve describing the conformity of $\beta_{\text{loc}}$ at the top of the model CNT to the radius of the hemisphere $R$.

FEF at the top of the CNT was calculated by dividing the local field $E_{\text{max}}$ (the field at the top of the cylinder) by the macroscopic field $E_M$

$$\beta = \frac{E_{\text{max}}}{E_M}.$$  

(5)
The distribution of the field enhancement factor $\beta$ over the surface of the model nanotube with it's maxima value is shown in Fig. 5.

The resulting dependence $R(\beta)$ was approximated by a polynomial of the third degree:

$$R = 5.53 \cdot 10^{-8} \beta^3 - 2.21 \cdot 10^{-4} \beta^2 + 0.3 \beta - 140.82,$$

the graph of which is shown in the inset of Fig. 6.

The substitution of experimental $\beta_{\text{loc}}$ in this approximated dependence made it possible to transform them into a distribution of the radii of the hemispheres (Fig. 6), on which the model CNTs of the same height $h = 2.5 \mu m$ and radius $r = 1 \text{ nm}$ will be located. The interval for varying the radii of the hemispheres $R$ starts from 4 and ends at 12 $\mu m$.

The obtained data on the spatial distribution of the emission sites and the radii of the hemispheres $R$ allow us to proceed to the procedure for constructing the model surface of the SWCNT/P.

3. Construction of the effective surface of a multi-tip emitter

In the procedure for constructing a surface model, integration with the MATLAB programming package was used, which appeals to all parameters and elements of the COMSOL model through a special scripting language. First, the data on the spatial arrangement of the sites and the radii of the hemispheres $R$, obtained by translating the field enhancement factors $\beta_{\text{loc}}$, are read. As a result of executing the cycles of the MATLAB program code, the model surface has the form shown in Fig. 7.

A fragment of the model surface of the SWCNT/P on an enlarged scale, showing the spread in size of hemispheres and their mutual overlapping in the case of a close arrangement, is shown in Fig. 8.

![Figure 7](image1.png)  
**Figure 7.** Model of the SWCNT/P, constructed from hemispheres and model CNTs located on them.

![Figure 8](image2.png)  
**Figure 8.** Fragment of the model surface of the SWCNT/P on an enlarged scale.

Thus, our model emitter acquires an effective surface that is equivalent to the real specimen from the point of view of the location of the emission sites and the attainment of field enhancement factors on them.

Implementing model problems on the constructed effective surface requires large computational resources, since the number of finite elements required for the discretization of the model is large. Therefore, it has been decided to simulate the emission properties of individual sections of the emitter having the greatest density of the location of the emission sites.
Conclusion
We constructed the effective surface of a multi-tip field emitter by applying a multistage processing of the experimental data. Despite the primitiveness of the proposed model, in contrast to many more complex model systems that take into account the different subtleties of field cathode operation, the developed technique is related to experiment and can later evolve, including increasingly complex corrections.

The developed approach opens wide opportunities for establishing the mechanisms of the influence of various factors on the operation of the field cathode and qualitative prediction of the evolution of its emission characteristics. The constructed effective surface of real LAFE allows to carry out various computer calculations based on it: to investigate the influence of the mutual screening effect on the nature of the total emission current, to calculate the temperature distribution on the emitter surface, to simulate adsorption-desorption processes, and also ion bombardment affecting the emission properties of LAFE.

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