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Optimization for field emission from carbon nanotubes array in hexagon

Xin-Qing Wang [a,b,*], Ya-Bo Xu [c], Hong-Liang Ge [a,b], Miao Wang [c]

[a] *Department of Physics, China Jiliang University, Hangzhou 310018, China*
[b] *Zhejiang Province Key Laboratory of Magnetism, China Jiliang University, Hangzhou 310018, China*
[c] *Department of Physics, Zhejiang University, Hangzhou 310027, China*

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Abstract

In order to investigate the influence of the arrangement of the carbon nanotubes (CNTs) array on the field emission, the more practical model in hexagon was proposed. From the calculation with the image floated sphere model, the results showed that the arrangement has little influence on the field emission and the intertube distance R of CNTs array critically affects the field emission from the CNTs array, which accords with the results from the numerical simulations and experiments. When R is less than the height of tube h, the enhancement factor decreases rapidly with R. Considering the field emission current density, the field emission can be optimized when R is comparable with h, which accorded with the results from experiments. Furthermore, the influence of the anode–cathode distance d on the field emission from CNTs array was also discussed, which proved that d has little effect on the field emission from CNTs array. For the fixed field strength E for the certain materials in filed emission, we can reduce the threshold voltage to some extent by decreasing d in the case of $R>2h$.
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Keywords: Carbon nanotube (CNT); Field emission; Enhancement factor; Field emission current density; Hexagon

1. Introduction

Carbon nanotubes have attracted considerable attention due to their unique geometry, the excellent structure and prominent electronic properties, which demonstrate the potential application in many fields [1–3], especially in the field of field emission displays [4–6]. The CNTs have the diameter of the order of nanometer and up to a few micrometers length. The nanoscale tip and the higher aspect ratio h/ρ (ρ is the radius of CNTs) lead to the greater local field at the tip of CNTs, and the emission electrons could easily penetrate the potential barrier into the vacuum with tunnel effect with a low emission threshold voltage [7,8], then the higher current density could obtain with a lower emission threshold voltage. Therefore, it is not surprising that CNTs are considered to be ideal candidates for the next generation field emitters for flat panel displays, field emission electron source, microwave power amplifiers and so on [9–11].

Studies have shown that many parameters, including the gas molecule, the microstructure of the top, h/ρ, d, R, the CNT with open/close cap and so on, can influence the field emission properties of the CNTs array [12–17,22,23]. If all the above parameters were taken into account, an approximate analytic solution for the field emission from CNT or CNTs array and the variation trend of the field emission versus the different parameters could not be obtained. Simulation and calculation for the field emission from CNTs with the simplified models are mainly concentrated on an individual CNT [17,18] or several CNTs [19]. Buldum and Lu [7] obtained the local potential energy around the top of CNT by solving Laplace's equation numerically and calculating the effective electronic potential using self-consistent field (SCF)-pseudopotential electronic structure calculation method. In our previous paper [18], the floated sphere model was proposed to calculate the field enhancement factor for an individual CNT, and the results showed the good properties of field emission from CNT is attributed to the very large h/ρ and d has little influence on the field enhancement factor of individual CNT. Mayer et al. [19]

* Corresponding author. Department of Physics, China Jiliang University, Hangzhou 310018, China.
E-mail addresses: wxqnano@cjlu.edu.cn, wangxinqingnano@163.com (X.-Q. Wang).

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had researched the field emission from bundles of metallic (5,5) CNTs, and found the enhancement factor of individual CNT to be larger than that of CNTs array due to the electrostatic interactions between CNTs.

In field emission devices, however, the CNTs are not mostly individual but often grown in arrays or entangled form. And many experiments [14–16] had proved that R critically affects the field enhancement factor of CNTs array, which had stated that the field emission could be optimized when R is comparable with h. Furthermore, the field emission from the CNTs array [20] in square was also studied theoretically with the floated sphere model and the expression of the enhancement factor could be expressed as $\beta=h/\rho+3.5-W$ (W is the function of R), which proved that the field enhancement factor of CNTs array is approached to the maximum $\beta=h/\rho+3.5$ when R is much larger than h. If the field emission current density was taken into account, the field emission could be optimized when R is close to h, which accorded with the others' results [14–16].

In this paper, with the model of floated spheres and the image method described in the previous paper [18,20], an approximate analytic solution for the CNTs array in hexagon can be obtained and the enhancement factor was modified to be as $\beta=\frac{h}{\rho}\left(\frac{1}{1+Y}\right)+\frac{1}{2}\left(\frac{1}{1+Y}\right)^2+3$, which Y is the function of R. And the results showed that the arrangement has little influence on the field emission and R greatly affects the performance of the field emission from CNTs array. Furthermore, d was introduced into the calculation, and the results showed that the field emission from CNTs array hardly changes versus d. Thus, we can easily illustrate the variation trend of the field emission versus the different parameters including R and d.

2. Modeling and calculations

With the model of floated spheres and the image method described in the previous paper [18,20], the model system of the CNTs array in hexagon was shown in Figs. 1 and 2. We assume the CNTs are conducting, the cathode potential is maintained zero over whole its surface. In accord with the practical CNTs array, we assume $\rho \ll h$ and $\rho \ll R$. Thus we can keep only the first order terms of r/R and r/h in any expansion. In the first step, we consider only the case when $d \gg h$. In this case, the potential near a specific floated sphere with its center at the origin O can be considered as produced by the two layers of point charges array (each point with charge Q or $-Q$) antisymmetrically situated above and below the cathode plane, together with a dipole $-P$ at O, which described in the previous papers [18,20]. The distance between the floated sphere at (x, y) and the origin O in Fig. 2 could be expressed as $R^2(x,y)=R^2(x^2+y^2+xy)$ according to the cosine law.

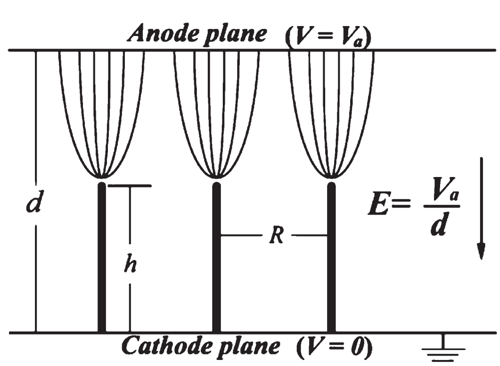

Fig. 1. The model for the field emission from the CNTs array.

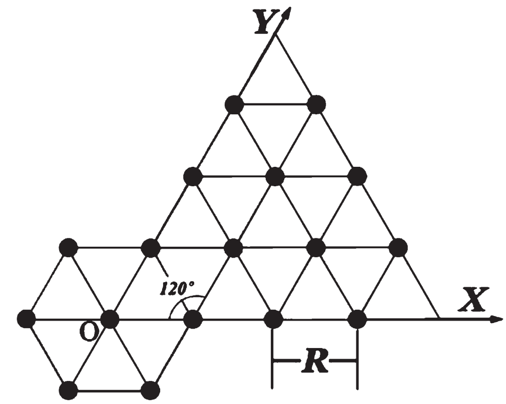

Fig. 2. The calculated model for the enhancement factor of CNTs array.

As mentioned in the previous paper [20], the contribution of all the first order of r/R and all the dipoles except the one situating at O can be neglected. Accurate up to the 1st order of ρ/h and ρ/R, the potential near O can be expressed as

$$\varphi(r,\theta)=\frac{-Q}{4\pi\varepsilon_0 r}\left(1-\frac{r}{2h}\right)+E_m h+\frac{-P}{4\pi\varepsilon_0 r^2}\cos\theta + E_m r\cos\theta+\frac{-QK}{4\pi\varepsilon_0 R}, \quad (1)$$

where the first four terms are the contribution of the charges at O and O′, E_m denotes the mean field strength between the anode and cathode. The fifth term represents the contribution of the others charges at the two layers expect the charges at O and O′. Different to the CNTs array in square, the nearest charges to O are six for the CNTs array in hexagon. If we assume $N=h/R$, the K in Eq. (1) could be expressed as $K=\sum_{x=0}^{L}\sum_{y=1}^{L}\left(\frac{6}{\sqrt{x^2+y^2+xy}}-\frac{6}{\sqrt{x^2+y^2+xy+(2N)^2}}\right)$, which is the function of R. Supposing $Y\equiv\rho K/R$, the requirement of $\varphi=0$ at the sphere surface ($r=\rho$) gives the following equations: $Q=4\pi\varepsilon_0 E_m h\rho\left(\frac{1}{1+Y}\right)\left(1+\frac{\rho}{2h(1+Y)}\right)$, $P=4\pi\varepsilon_0 E_m \rho^3$, where Y is always greater than zero. Substituting these into Eq. (1) and calculating the field strength at the top of the sphere at O, we obtained another expression of the enhancement factor of the CNTs array,

$$\beta=\frac{h}{\rho}\left(\frac{1}{1+Y}\right)+\frac{1}{2}\left(\frac{1}{1+Y}\right)^2+3 \quad (2)$$

The above calculation has been carried out assuming d to be infinite compared to h. In the following paragraphs, the influence of d on the field emission from CNTs array in hexagon was studied in the same way as in the previous paper [18,20].

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