Exact field enhancement factor, electrostatic force and field emission current from a long carbon nanotube

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ABSTRACT

Field enhancement factor, electrostatic force and field emission current from carbon nanotube film are theoretically investigated. In our model the cathode resembles a dense carpet consisting from randomly twisted nanotubes. Under the action of electric field the free ends of nanotube are built in parallel lines of intensity of a field. Emitting tubes come off at the certain electrostatic forces. The further voltage increase causes other tubes to emit till the force is still insufficient to tear them off of a substrate.

Keywords: carbon nanotubes, field emission, electrostatic force

1 INTRODUCTION

After experimental discovering of fullerenes [1] and carbon tubes [2] many researches are devoted to studying of their properties and possible applications. One is easier to imagine nanotube by mental folding of a graphite layer. As a result of such action the seamless open cylindrical tube should turn out. Closed nanotubes are ended with hemispherical caps.

Remarkable properties of carbon nanotube films is their ability to act as field emission electron sources at low applied voltages. Now field emission arrays on the basis of carbon nanotube films for field emission displays are developing.

The key problems restricting large-scale industrial use of cathodes on carbon nanotube films is the problem of lifetime and reliability.

We assume one of aspects of this problem consists that during emission in strong electric fields the part of tubes is pulled out from a film and adheres to the anode [3].

2 EXPERIMENTAL DATA

We investigated films obtained by various technologies of synthesis. Fig. 1 shows the I-V characteristic of the film. It is visible that at a direct current 250 µA a reverse current appears and at a direct current 500 µA it reaches 20 µA. Occurrence of a reverse current also confirms that nanotubes come off from the cathode and adhere to the anode. The assumption about pulling out of nanotubes was reported elsewhere [2-3].

Figure 1: I-V characteristic of the film.

3 THEORETICAL CALCULATIONS

Let's consider how to explain tubes detaching from a substrate and what forces hold these tubes.

3.1 Electrostatic forces acting on a nanotube

During field emission electrostatic force acts on a tube and aspires to tear off it from a substrate. For numerical calculation of a field emission from aligned carbon nanotube we use the following model:

1. The nanotube is a cylinder with length $H$ and diameter $d$ that is closed with a hemispherical cap with the same diameter $d$.

2. Nanotube obeys the laws of continuous medium, it is an ideally conducting material and the cathode potential is maintained at its whole surface.

For numerical calculation we used special finite-element technique [3].
In case \( L \gg H \) the field amplification factor is well described by the formula

\[
\beta = 3 + Bx^D
\]  

(1)

where \( x = H/d \); \( B = 2.372 \); \( D = 0.8562 \). Parameters \( B \) and \( D \) were evaluated using least squares method.

Distribution of the electrical field intensity on the hemispherical nanotube cap was fitted as following:

\[
E = E_{\text{max}} (1 - A_u a^2)
\]  

(2)

where \( E_{\text{max}} = \beta E_0 \) is the maximum electrostatic field at the apex of the nanotube and \( E_0 \) is the applied macroscopic field, i.e., the far-field, \( \alpha \) is a minimal angle between radius to a point on hemisphere and nanotube axis, parameter \( A_u = 0.1288 \). Angle \( \alpha \) is measured in radians \( 0 \leq \alpha \leq \pi / 2 \). Noticeable field emission may be observed from approximately half of nanotube cap, the rest of emission current is negligible.

Consider force stretching vertically oriented nanotube.

Using the formula (2) it is possible to find the electrostatic force stretching a single tube, perpendicularly oriented to a substrate [3]

\[
F = 8.26 \varepsilon_0 E_{\text{max}}^2 \pi r^2 / 2
\]  

(3)

where \( E_{\text{max}} \) is maximal electric field (V/\( \mu \)m); \( r \) is tube radius (Å); \( \varepsilon_0 \) is electric constant (F/m); \( F \) is force (nN), and 8.26 is dimensionless factor.

As schematically shown in Fig. 2 our carbon films represent dense "carpet" from randomly oriented nanotubes. We suppose that under the action of electric field the free ends of nanotube are built in parallel lines of intensity of a field. Thus a film from randomly oriented nanotubes converts into the array of aligned nanotubes (see Fig. 2). Force (3) acts to nanotube apex and aspirs to extract a tube from "carpet". The tube is kept by van der Waals interaction with other tube.

![Image](image.png)

Figure 2: "Carpet" from randomly oriented nanotubes.

### 3.2 Van der Waals forces for nanotubes

For van der Waals forces calculation we use Lennard-Jones potential well describing interatomic interactions.

\[
\varphi_a(r) = B / r^{12} - A / r^6
\]  

(4)

Parameters of potential \( A = 15.2 \text{ eV}\cdot\text{Å}^6 \) and \( B = 24.1\cdot10^3 \text{ eV}\cdot\text{Å}^{12} \) for C-C interactions in graphite planes are taken from work [7]. As we believe, nanotube is kept due to interaction with other tubes, thus using of carbon-carbon potential in calculations is quite justified.

We used method [8] of potential integration over tube surfaces to get single wall tubes van der Waals potential. Then it can be generalized by summation over different interacting walls to potential of multi-wall nanotubes. We was able to get exact analytical formula for van der Waals potential and force \( f_{\text{c}}(t_x, t_y, x) \) between carbon multi-wall nanotubes at radius \( t_x, t_y \) and distance \( x \). Full analytical formula and derivations are quite huge, so we would like present here only potential between two single wall tube at the same radius.

\[
\varphi_{\text{c}} (r, t) = -2 \pi \left( \frac{A f_a}{r^6} + \frac{B f_k}{r^8} \right),
\]

(5)

\[
\lambda = \frac{2 \sqrt{t_1 t_2}}{\sqrt{r + t_1 - t_2} \sqrt{r + t_2 - t_1}},
\]

(6)

\[
f_k = f_{\text{ak}} K(\lambda) + f_{\text{ak}} E(\lambda),
\]

(7)

where \( K \) and \( E \) are complete elliptical integrals of first and second kind.

\[
f_{\text{ak}} = -2(5\chi^2 - 4) / 3(\chi - 2)^2(\chi + 2)^2, \quad \chi = \frac{r}{t},
\]

(8)

\[
f_{\text{ae}} = 2(32 - 20\chi^2 + 11\chi^4) / 3(\chi + 2)^2(\chi - 2)^5,
\]

(9)

\[
\begin{align*}
4609\chi^{14} + 56038\chi^{12} + 321132\chi^{10} - \\
473632\chi^8 + 1885952\chi^6 - 3867648\chi^4 + \\
4510720\chi^2 - 2293760
\end{align*}
\]

(10)

\[
/1575(\chi - 2)^8(\chi + 2)^8,
\]

(11)

\[
\begin{align*}
7129\chi^{16} + 97220\chi^{14} + 763489\chi^{12} - \\
1533424\chi^{10} + 7790944\chi^8 - \\
21756160\chi^6 + 38781184\chi^4 - \\
40099840\chi^2 + 18350080
\end{align*}
\]

(11)

Potential derivation gives required van der Waals force. Investigating this derivative on extreme, it is possible to
find distance on which van der Waals interaction will be maximal.

\[ F(r) = \max_x F_w(r, r, x) \]  

(12)

In figure 3 we show dependence of maximal force (nN) on tubes radius (Å).

![Graph showing dependence of maximal van der Waals force on tube radius.]

Figure 3: Dependence of maximal van der Waals force on tube radius.

Using (1), (3) and \( F(r) \) (Fig. 3) we get

\[ H(E, r) = 2 \left( \frac{1}{B} \frac{1}{Er} \sqrt{\frac{2F(r)}{8.26\varepsilon_0}} - 3 \right)^{1/D} \]  

(13)

In figure 4 for different values of applied electrical field we draw \( H(\theta) \) divided space \((H, r)\) into two regions. In the upper region tubes having one contact with other tube at the same radius will be detached. Otherwise it will be held by van der Waals force for the down region.

![Graph showing critical curve for given electrical field.]

Figure 4: Critical curve \( H(\theta) \) for given electrical field.

In figure 5 we have similar “break lines” for different given tube diameters that predict dependence of critical height on applied electrical field.

In this work the electrostatic forces acting on a nanotube are calculated. Using the Lennard–Jones potential the van der Waals forces keeping tubes on a substrate are estimated. Tubes detachment conditions are being analyzed.

4 CONCLUSION

REFERENCES