Numerical calculations on the field emission of carbon nanotubes

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Numerical calculations on the field emission of carbon nanotubes

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Abstract. Carbon nanotubes (CNTs) have been proven experimentally to be well suited for field emission applications. However, the exact process of electron emission from CNTs is still not fully understood. In this paper, we numerically investigate the effects of electrostatic field screening at the CNT emitter tips by finite element method and show the impact on device performance. We further observe that to achieve maximum emission efficiency of CNTs in an infinite line, one need to have an intertube distance of three times the CNT height. These results can be used to develop an optimized CNT field emission array that fits within the constraints of currently available fabrication capabilities.

1. Introduction
Since Iijima published his seminal article in Nature identifying multi-walled carbon nanotubes in 1991, Carbon nanotubes (CNTs) have attracted tremendous interest from fundamental science and technological perspectives [1]. CNTs posses many unique properties due to their low dimensionality make them promising candidates for future technology applications. CNTs have been used in many laboratories to build prototype nanodevices. Understanding these novel properties and their impact on devices is crucial in the development and evolution of CNT applications.

CNTs have been proven experimentally to be well suited for field emission applications. This is related to that CNTs have many unique properties such as narrow diameters, high aspect ratios, high temperature stability, good conductivity and structural strength. Prototype devices using the superior field emission properties of CNT have been demonstrated. These devices include x-ray tubes [2], scanning x-ray sources [3], flat panel displays [4, 5] and lamps [6]. CNTs make excellent electron emitters not because of a low work function but due to the extremely high local electric field that forms at the small diameter tips.

The ability to grow aligned CNTs on a substrate has made it possible for designers to specify the height, radius, separation, etc. However, the exact process of electron emission from CNTs is still not fully understood. Much work has been done on the emission process through experimental and numerical investigations for further understanding [7, 8]. It has long been assumed that the field screening is negated when adjacent emitters are at a separation of twice their height [9]. In this paper, we investigate the effect of electric field screening on an infinite line of CNTs by means of two-dimensional simulation and show the impact on the device performance.

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2. Numerical model and results

CNTs were simulated in 2D by solving the Laplace equation with finite element method (FEM). The simulation allows the extraction of potential and electric field at any point around the structure. The schematic diagram of simulated line of CNT is shown in the figure 1(a). The CNTs are treated as perfect conductors in our model. Vertically aligned CNTs of uniform height $h$ and radius $r$ are placed on a grounded cathode that is separated from the positive anode by distance $D$. The intertube distance is denoted as $d$. Field emission occurs primarily due to the physical dimensions of CNTs. CNTs can range from 0.6 nm to more than 100 nm in diameter and tens of nanometers to microns and even millimeters in length resulting in incredible aspect ratios. We assumed tubes of 1 $\mu$m length with a tip apex of 2 nm in our calculation the same as previous reported in Nilsson’s work [10]. The resulting focus of the electric field at the tips of the CNTs is often referred to as the electric field enhancement factor $\beta$ which depends on the geometry of the tip. The field enhancement will increase for smaller diameter CNTs and decrease for larger diameter CNTs.

![Figure 1(a)](image1a.png)

**Figure 1.** (a) Schematic of the simulation setup of a line of CNTs of height $h$ and radius $r$ placed on a grounded cathode and beneath an anode at a distance of $D$; (b) The simulation shows the equipotential lines of the electrostatic field with the background surface indicating the magnitude of the electric field. The CNTs used here have height of $h=1$ $\mu$m and radius of $r=2$ nm, the intertube distance is $d=0.5$ $\mu$m.

A simple 2D simulation of 3 element CNT line with intertube distance of 0.5 $\mu$m was first used and the calculation results were shown in the figure 1(b). The equipotential lines of the electric field with the background surface of the magnitude of the electric field are depicted. The anode is located relatively far away from the CNT emitters so its contribution to the electric field is assumed to be small and uniform. According to our calculation, the electric field at the central tube is lower than that of the outer tube. This is explainable by an electrostatic screening effect provoked by the proximity of neighbouring tubes. The CNTs are too close together for electrostatic field penetration which negates some of the expected field enhancement. These electrostatic screening effects are clearly evident in the simulation results shown in figure 1(b). Nilsson et al conducted a study of screening effects by performing 2D simulations of field penetration and the optimized separation between individual CNTs was determined to be twice the CNT height [10]. 3D simulations performed by Smith et al showed 2D simulations underestimated the effects of screening and determined an optimized separation of 3 times the height of the individual CNTs [11].

To investigate the electric field screening effect as a function of intertube distance, we simulate an infinite line of CNTs with periodic boundary condition. The intertube distance ranged from 0.1 $\mu$m to 6 $\mu$m in our calculation, which corresponds to the ratio $d/h$ of 0.1 to 6. The local electric field was carefully extracted at the point immediately above the CNT tip. The percentage of screening was calculated by the difference in the local electric field to that of an identical but isolated CNT. Figure 2 shows the percentage of screening as a function $d/h$ for CNT of radius 2 nm, height 1$\mu$m. We can see that the amount of screening decreases as $d/h$ increases. The amount of screening at $d=2\ h$ indicates...
that there is a 4.3% drop in the local electric field. When the intertube distance increased to \( d=3h \), the drop of screening falls to 1.1% which means the CNT is performing at 99% of its optimum value. The percentage of screening was found to be 0.2% when the intertube distance is further increased to \( d=4h \). To achieve a fully unscreened line of CNT, one needs to have an intertube distance in excess of three times the height of CNT.

![Figure 2](attachment:figure2.png)

**Figure 2.** Percentage of electrostatic screening as a function of intertube distance over CNT height calculated by the difference in the local electric field between an isolated CNT.

It is important to consider the effect of screening in maximizing the current. Perhaps the most obvious approach to increasing the current density is to decrease the intertube distance. This will increase the number of emitters across the line resulting in a higher total current density, as long as the reduced intertube distance does not cause screening effect between neighbouring CNTs. The current density is calculated using the well known and widely accepted Fowler-Nordheim equation

\[
J = \int \frac{aE^2_L}{\phi} \exp \left( \frac{-b\phi^{3/2}}{E_L} \right) \, ds
\]

where \( a \) and \( b \) are constants with values \( 1.54 \times 10^{-6} \text{ AeV}^{-2} \) and \( 6.83 \times 10^{3} \text{ eV}^{-3/2} \text{V} \mu \text{m}^{-1} \), respectively. \( E_L \) is local electric field in \( \text{V} \mu \text{m}^{-1} \) at the surface of CNT and \( \phi \) is the work function with value 4.5 eV. The integration is calculated over the CNT surface.

We calculated the emission current density for an infinite line of CNT and the result is plotted in figure 3. We observe a sharp increase in current density as the initially tightly packed CNTs become more separated. The current density reaches maximum when the intertube distance approaches three times the CNT height. Beyond this value, the current density decreases. This is because the far separated CNTs have very few efficient emitters while the closely packed CNTs suffer from electrostatic screening due to the neighbouring nanotubes. The nearly linear decrease beyond \( d=3h \) would be expected, as at these intertube distance each emitter is unscreened, i.e., half the CNT equals half the current density. The most efficient arrangement of CNTs in a line, for maximizing the current density, is \( d=3h \), giving rise to a 1.1% screening of the local field.
Figure 3. The calculated field emission current density of CNT with height 1 µm and radius 2 nm as a function of d/h.

3. Conclusions
In conclusion, we have simulated an infinite line of CNT emitters and investigated the effect of field screening in terms of intertube distance. We found that the optimum intertube distance needs to be in excess of three times the height of the CNT to achieve a fully unscreened line. Our calculations predicate that an intertube distance of three times the CNT height optimizes the emitted current density.

Acknowledgments
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