Optimization of Carbon Nanotube Field Emission Arrays

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Abstract: Carbon nanotubes (CNTs) have been proven experimentally to be well suited for field emission applications. An optimized triode configured CNT field emission array is developed using the COMSOL Multiphysics Electrostatics Application to adjust five key physical dimensions to investigate the effects on the enhanced electric field at the CNT emitter tips. The five dimensions studied are CNT spacing, array pitch, array element dimensions, element shape, and the dielectric thickness. These results are used to develop an optimized CNT field emission array that fits within the constraints of currently available fabrication capabilities.

Keywords: carbon nanotube, field emission arrays.

1. Introduction

Since Iijima published his seminal article in Nature identifying multi-walled carbon nanotubes in 1991, research into the properties and applications of carbon nanotubes (CNTs) has flourished [1]. In 1995, only four years after carbon nanotubes were introduced to the scientific community by Iijima, de Heer *et al* demonstrated the field emission capabilities of carbon nanotubes with the fabrication of a small electron gun using multi-walled carbon nanotubes [2]. CNTs have many unique properties ideal for field emission such as narrow diameters, high aspect ratios, high temperature stability, good conductivity, and structural strength. Carbon nanotubes 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. CNT field emission devices are created in two configurations, diode and triode. The diode configuration uses CNTs as the cathode and a conductive anode for extraction and collection of emitted electrons. The triode configuration, shown in Figure 1, uses CNTs as the cathode, a gate for extraction, and a conductive anode for collection. A triode design is preferable to a diode design for arrays primarily because the extraction voltage required is much lower due to the proximity of the gate to the CNTs. A triode design also has the potential to reduce screening effects which limit electron emission to a small fraction of the CNTs within the extraction electric field. Carbon nanotube synthesis technology provides a method to control CNT height and to a minor extent areal density. The array element shape, dimensions, and pitch can be controlled through standard fabrication processes. This research effort uses COMSOL simulations to develop an optimized design for a gated CNT field emission array within the currently available fabrication capabilities.

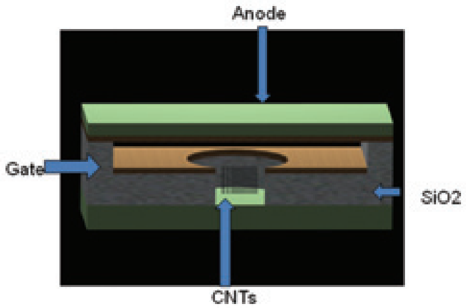

Figure 1. Schematic of triode configured CNT field emission device.

The goal is to obtain high array current densities by maximizing the electric field strength at the tips of the CNTs by balancing the array element dimensions, pitch, and height. The effects of CNT separation on the electric field intensity are also simulated.

2. Carbon Nanotube Array Models

As mentioned above, there are a variety of properties that make CNTs well suited for field emission applications. However, field emission occurs primarily due to the physical dimensions of CNTs. Single walled CNTs have diameters from 0.6 nm to 1.4 nm and multi-walled CNTs can range from 12 nm to more than 100 nm in diameter. Both types of CNTs can range from tens of nanometers to microns and even millimeters in length resulting in incredible aspect ratios. The resulting focus of the electric field at the tips of the CNTs is often referred to as the electric field enhancement factor. Previous research as summarized by Bonard *et al* has shown multi-walled CNTs to be more robust emitters than single walled CNTs [3]. Multi-walled CNTs are also much easier to fabricate reliably, as such only multi-walled CNT dimensions are used in these models. While the conductivity of single walled CNTs can be metallic or semiconducting depending on the nanotube structure, all multi-walled CNTs are considered metallic conductors. With the physical geometry providing the primary enhancement of the electric field, the CNTs are treated as perfect conductors in the models.

A simple 2D model of a 1 x 3 element CNT array was used to investigate general trends, which were then confirmed with much more computationally complex 3D models. The initial 2D model, shown in Figure 2, was based on a previously developed fabrication process that consisted of a silicon (Si) substrate with a 200 Å titanium (Ti) diffusion layer followed by 100 Å nickel (Ni) catalyst layer. The nickel was covered with 2 µm of silicon dioxide (SiO_2) with 0.5 µm chrome gate metal on top. The array consists of 1 µm circular or square elements etched in the gate metal and SiO_2 with a 1 µm pitch. The anode is located directly above and relatively far away (10-50 µm) from the CNT emitters so its contribution to the electric field is assumed to be small and uniform in nature. Thus, the anode is not included in the model.

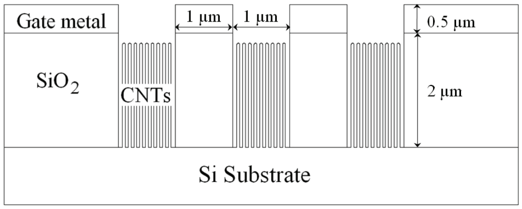

Figure 2. Basic 2D model of 1 um x 3 gate array with 1 um pitch.

The CNT films grown from the Ni catalyst via microwave plasma enhanced chemical vapor deposition result in closely packed CNTs with diameters of a fairly dispersive range, 10 - 100 nm. The process target is an average diameter of 50 nm, which is the diameter used in the simulations. The field enhancement will increase for smaller diameter CNTs and decrease for larger diameter CNTs.

Perhaps the most obvious approach to increasing the current density of an array is to decrease the array pitch. This will increase the number of elements across the array resulting in a higher total array current density. The effects of decreasing the spacing between gate openings was investigated by simulating 2D models with pitches of 3 µm, 2 µm, 1 µm, and 0.5 µm for both 1 µm and 0.5 µm array elements. Three dimensional simulations were also performed using 3x3 element arrays with 1 µm and 0.5 µm pitches.

The proximity of the gate to the CNT directly affects the electric field intensity. Thus, it's expected that decreasing the element dimensions will result in increased field strength. The trade-off is fewer CNTs within the smaller element. However, within a given element only a fraction of the CNTs are expected to emit at any given time. This is caused by electrostatic screening which is described in detail below. Experimental results with decreasing larger element dimensions from 18 µm to 4 µm have shown increased field emission current densities [6]. The smallest feature size available in the current fabrication process is 0.5 µm, so the electric field strength of 1 µm and 0.5 µm array elements were compared. 3D models were also created to compare the field strength of 1 µm and 0.5 µm circular and square elements. However, it should be noted that the current process is capable of only 0.5 um circular elements.

When de Heer *et al* first published the results of the first CNT field emission device, it was estimated that a mere 0.1 % of the total CNTs were emitting electrons. Initially, this was attributed to the geometry of the CNTs, it was assumed only a tiny fraction were sharp enough for field emission. It is now accepted that this phenomenon is caused by electrostatic screening. The CNTs are too close together for electrostatic field penetration which negates some of the expected field enhancement. Nilsson *et al* conducted a study of screening effects for diode configured CNTs by performing 2D simulations of field penetration [4]. An optimized separation between individual CNTs was determined to be twice the CNT height. 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. Neither of these optimized solutions is practical for gated arrays. Screening effects within the elements are unavoidable as the density of the CNTs can only be mildly influenced during the synthesis process. Although, the CNT spacing within an element was simulated at 50 nm, 200 nm, and with a single CNT to confirm electrostatic screening effects.

The limited electrostatic field penetration between densely grown CNTs introduces the possibility of improving the fabrication process by reducing the thickness of the dielectric layer and the height of the CNTs without any adverse effect on the electric field strength. As the feature sizes decrease; fabrication, especially etching, becomes more difficult unless there is a corresponding decrease in layer thicknesses. The dielectric thickness was simulated at 2 µm, 1 µm, and 0.5 µm with the CNT height adjusted accordingly. A dielectric thickness of 0.5 µm is probably not feasible due to the difficulty in reliably controlling CNT height below 0.5 µm.

Using the models and simulations discussed above, the optimization process can be summarized by varying these five parameters:

- CNT spacing
- array pitch
- array element dimensions
- element shape
- dielectric thickness

3. Use of COMSOL Multiphysics

The COMSOL electrostatics of dielectric materials application was used to simulate the electric field generated by the gate extraction voltage across the CNTs within the array elements in both 2D and 3D. The models were created by subtracting the conductors (substrate, CNTs, gate) from a surrounding dielectric block of air and silicon dioxide. Subdomain properties were used to set the silicon dioxide permittivity at 3.9. Boundary conditions were used to ground the substrate and CNTs and put a 1 V potential on the gate metal. Results were best visualized using contour and surface plots, while peak electric field magnitudes were recorded using point evaluations.

4. Simulation Results

Previous experimental and computer simulation research with diode configured CNTs indicated that relatively large spacing between the CNTs is necessary to avoid screening effects. These electrostatic screening effects are clearly evident in the simulation results shown in Figure 3. This simulation is of a 1 µm element with CNT spacing of 50 nm, 200 nm, and a single CNT in the center of the element. The simulation shows the equipotential lines of the electrostatic field with the background surface indicating the magnitude of the electric field.

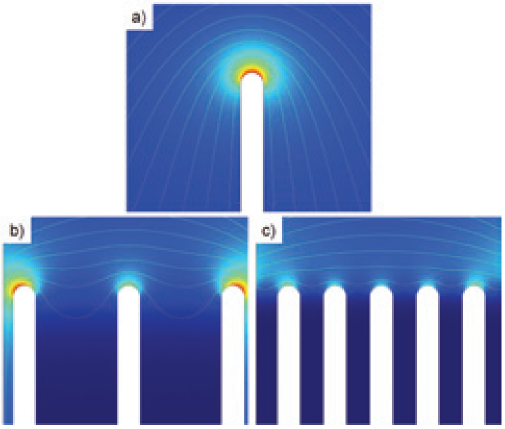

Figure 3. Screening effects for a) single CNT, b) 200 nm spacing, and c) 50 nm spacing.

The single CNT, shown in Figure 3 (a) clearly sees the most field penetration and correspondingly has the strongest electric field. There is a 42% reduction in electric field strength from the single CNT to the center CNT in Figure 3 (b) with neighboring CNTs 200 nm away. The magnitude of the electric field of the center CNT in Figure 3 (c) with 50 nm spacing is 60% less than the single CNT. The CNT spacing within each element cannot be controlled precisely, so the electrostatic screening within each gate is unavoidable at this time.

Decreasing the array pitch poses the simplest method to increase the total current density of the array, as long as the reduced pitch does not cause screening effects between array elements.

Results of array pitch simulations where the pitch of 1 µm and 0.5 µm element arrays were reduced from 3 µm to 0.5 µm are shown in Figure 4. The magnitude of the E-field at the tip of each CNT at each pitch are plotted. There is no reduction in magnitude across the center of each array element where the screening effects of immediately neighboring CNTs dominate. The 0.5 µm pitch causes a small reduction (~4%) in the E-field magnitude of the edge CNTs.

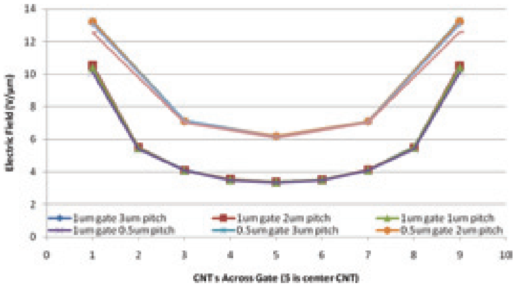

Figure 4. E-field magnitude at CNT tips of 1 µm and 0.5 µm element arrays with varying pitches.

3D simulations of a 3x3 0.5 µm element array with 1 µm and 0.5 µm pitches yielded similar results. Figure 5 shows the 3D model and the resulting E-field magnitudes at the CNT tips of the center element. The scales are identical for both surface plots and show no discernable difference between the two pitches. Quantitative analysis across the entire array resulted in only a 2 % difference between the two arrays. Reducing the array pitch has little affect on the magnitude of the electric fields generated across each element; while the increased number of elements will result in larger total array current densities.

Reducing the array element dimensions has the potential to increase over all array current density in two ways. First, smaller elements will increase the total number of elements across the array. Second, as shown in Figure 4, the decreased distance between the CNT emitters and the gate increases the electric field. The center CNT electric field magnitude increases almost two fold from 3.3 V/µm to 6.1 V/µm with the reduction in element dimension from 1 µm to 0.5 µm.

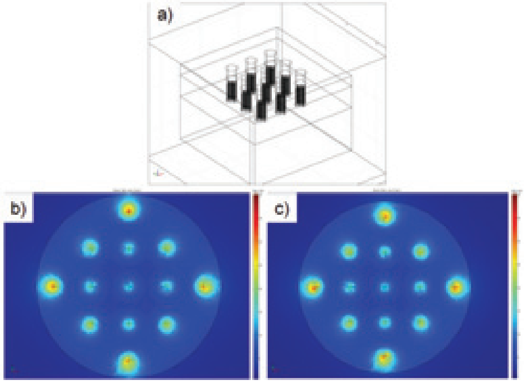

Figure 5. (a) 3x3 0.5 µm gated array with cross-section of E-field magnitude at CNT tips of the center element for (b) 0.5 µm and (c) 1 µm pitch.

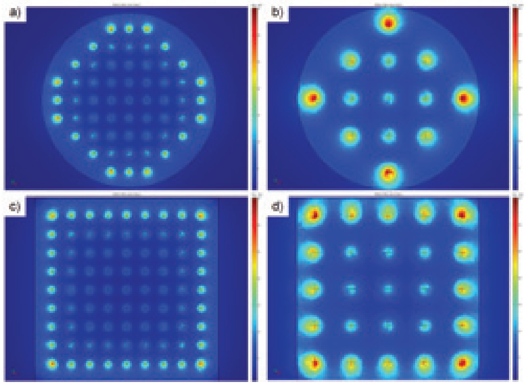

Figure 6. Cross-section of E-field magnitude at CNT tips of (a) 1 µm circular, (b) 0.5 µm circular, (c) 1 µm square, and (d) 0.5 µm square single elements.

Three dimensional simulation results comparing elements of 1 µm and 0.5 µm showed greater increases in electric field strength. The E-field magnitude at the CNT tips shown in Figure 6 clearly shows an increase for both circular and square elements when the element dimension is reduced. The center CNTs of the1 µm circular and square elements have E-field magnitudes of 5.3 V/µm and 7.8 V/µm respectively. The center CNTs for the 0.5 µm circular and square elements increases to 14.7 V/µm and 17.7 V/µm respectively. Both 3D and 2D results confirm an increase in the electric field across the element with decreasing element dimensions.

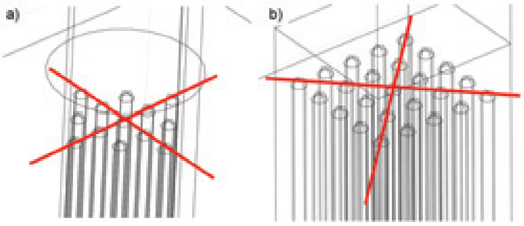

Figure 7. Comparison of E-field magnitude along similar diagonals of circular and square elements.

These simulations also provided a comparison between square and round element shapes. It is interesting to note that in all cases the center CNT of the square element has a slightly higher E-field. Comparison along similar diagonals, shown by the red lines in Figure 7, for both the 1 µm and 0.5 µm elements did not indicate a general increase in electric field strength. However, the square element has more CNTs with as strong and in the center slightly stronger electric fields than the circular element. This indicates that a square element is a better shape for the same feature size.

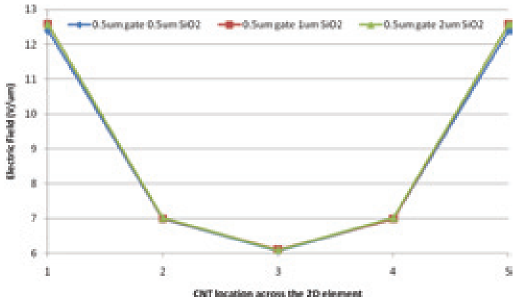

Figure 8. E-field magnitude at CNT tips across 2D element for dielectric thicknesses of 0.5 µm, 1 µm, and 2 µm.

Fabrication of small feature sizes, such as 0.5 µm elements with 0.5 µm pitch can be daunting when it requires etching through 2 µm of dielectric material. The last set of simulations compares the electric field across the 0.5 µm elements with 0.5 µm pitch when the SiO_2 dielectric layer is 2 µm, 1 µm, and 0.5 µm. The height of the CNTs is adjusted accordingly as well. Figure 4 shows a small reduction in the outside electric field strength at the 0.5 µm pitch due to element to element screening effects. After accounting for this slight reduction, results of 2D simulations in Figure 8 show no electric field degradation regardless of the SiO_2 thickness.

Corresponding 3D simulations of 3x3 arrays with 0.5 µm circular elements and 0.5 µm pitch are shown in Figure 9. Figure 9 (a) is the results for the 0.5 µm dielectric thickness and shows a slight decrease in the electric field from the other two cases. The magnitude at the center is ~10 % less with the edges decreasing by smaller amounts. There is virtually no difference between the 1 µm and 2 µm dielectric thickness results. Reducing the dielectric thickness to improve fabrication reliability should not degrade the field emission properties of the resulting arrays.

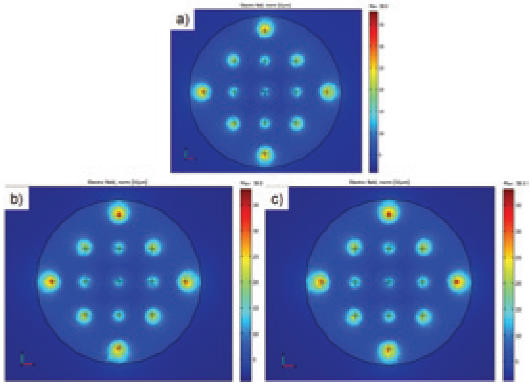

Figure 9. Cross-section of E-field magnitude at CNT tips of the center element of 3x3 array with SiO_2 thickness of (a) 0.5 µm, (b) 1 µm, and (c) 2 µm.

5. Conclusions

Carbon nanotubes have unique physical and electrical properties making them exceptional field emitters. COMSOL multiphysics has been used to optimize the physical dimensions for CNT field emission arrays. Five relatively simple parametric studies were performed to provide important insights into the design of field emission arrays within fabrication capabilities.

First and foremost, these simulations have shown that the electrostatic screening between CNTs within an array element is the dominating factor of the electric field magnitude. Any adjustments to the CNT synthesis process that can increase the carbon nanotube spacing will increase the electrostatic field penetration between CNTs and increase the local electric field magnitude. The screening effect is so dominant within the array elements that the pitch can be reduced significantly without adversely affecting the electric field magnitude at the CNT tips. Reducing the pitch will increase total array current density by increasing the total number of array elements. The same principle applies to the element dimensions. Reducing the element dimensions results in stronger electric fields and increases the total number of elements, both of which will increase overall current density. The simulation results of element shape showed that a square element will potentially provide a better array fill factor without degrading the electric field strength; making it a better choice over a circular element of the same diameter. Finally, due to the dominant screening effects, the dielectric layer thickness and CNT height can be reduced significantly without decreasing the electric field strength.

The resulting optimized CNT field emission array that fits within current fabrication capabilities at AFIT consists of a 0.5 µm circular element array with 0.5 µm pitch. The SiO_2 dielectric layer can be reduced to 1 µm with a corresponding CNT height between 0.5 µm and 0.8 µm. The simulation results indicated a square element will perform better than a circular element. However, due to limitations of the current fabrication process, a circular element is used in the final design. Figure 10 shows the basic two dimensional schematic of the final array design.

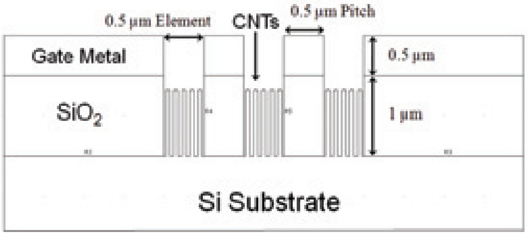

Figure 10. Optimized CNT field emission array basic schematic.

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