FEM Simulation of Nanotubes Manipulation Using Dielectrophoreseis

Vaibhav Mathur[1], Jin Li[1], Joel Therrien[2] and William D. Goodhue[*, 1]
[1]Photonics Center, Department of Physics and Applied Physics
[2]Department of Electrical Engineering
University of Massachusetts, Lowell, MA-01854
*720, Suffolk St., Lowell, MA 01854-3614, USA, William_Goodhue@uml.edu

Abstract Carbon nanotubes have emerged as a promising material in nanotechnology, electronics and optics for their excellent mechanical strength and unique electrical properties. Most researches in nanotubes manipulation have been focused on using the atomic force microscope (AFM). Recently, dielectrophoresis (DEP) was shown to be a useful technique for single nanotube manipulation and sorting of semiconducting-single walled nanotubes (s-SWNTs) from metallic-single walled nanotubes (m-SWNTs). The finite element method (FEM) (COMSOL package) has been employed here to model this phenomenon. In the FEM model, a pair of micro-electrodes is biased to generate a concentrated non-uniform electric field in an electrolyte in which SWNTs are dispersed. Two-dimensional (2-D) model of SWNTs are then created. The DEP force induced on the SWNTs by the electric field is computed in the AC/DC module and the resulting displacement is calculated in the coupled structural mechanics module. The displacement of the nanotubes as a function of the electrodes biasing and spacing, the orientation and electrical properties of the nanotubes are reported here. The simulated results will be used to guide the design of a novel micro-electro-mechanical system for carbon nanotubes sorting and deposition.

Keywords: Nanotubes, micro-electrodes, dielectrophoresis, FEM.

1. Introduction

It is widely recognized that carbon nanotubes will play an important role in future nano electronic devices. Field effect transistors (FET) using nanotubes as the semiconducting channel have demonstrated very high mobilities [1]. Metallic single walled nanotubes could find important applications such as electrical leads in nanoscale circuits [2]. The two major hurdles encountered in the full realization of these applications have been the lack of reliable techniques for single nanotube manipulation as well as in separation of semiconducting-SWNTs from metallic-SWNTs.

Several methods have been demonstrated for depositing nanotubes on microstructures, ranging from using an AFM [3] tip for single tube manipulation to chemically pre-patterning [4] the substrate. However, these techniques have a very low yield and poor reproducibility. Sorting techniques involving filtration and ultrasonication face similar issues. Recently, electric field assisted assembly utilizing dielectrophoresis has been shown to be much more effective in this regard. The magnitude and direction of the DEP forces on a nanotube are dependent on its electrical properties such as permittivity, conductivity which serve as a basis for sorting nanotubes [5]. Furthermore, DEP forces can be used to selectively deposit and manipulate nanotubes when they are subjected to high electric field gradients created by micro-electrodes [6].

The micro-electrodes device proposed here is similar to the optical micro-cantilever structure reported earlier [7]. The micro-cantilevers based on the AlGaAs material system are fabricated using a combination of lithography, dry and wet etch, and laser cutting techniques. The top epitaxial layer of the micro-cantilevers is heavily n-doped to serve as the electrodes. The device is then immersed in an electrolyte solution containing dispersed nanotubes. When the electrodes with optimal spacing are driven by an AC source in the RF frequency regime, the DEP force generated on the nanotubes can be utilized for sorting and deposition of the free floating nanotubes across them.

In the FEM simulation reported here, the in-plane movement of the nanotubes due to the

DEP forces is modeled in two dimensions. The electric field around the AC driven micro-electrodes is first solved in the AC/DC module and the gradient of the electric field is computed to determine the DEP force in the vicinity of the electrodes. This force is next applied on the nanotubes(s) as a sub-domain load in the structural mechanics module to model their movement. The mapped mesh is shown to be a handy tool here to mesh micro-electrodes and nanotubes with very high aspect ratio. In the simplified model here, the drag forces and Brownian motion of the nanotubes are neglected, as only the DEP force is predominant where it is very close to the microelectrodes [8].

2. Dielectrophoresis

2.1 Theory

Dielectrophoresis is the phenomenon in which a force is exerted on a dielectric particle when it is subjected to a non uniform electric field due to the induced dipole moment.

The DEP force exerted by the electric field $\vec{E}$ on a nanotube with the dipole moment $\vec{p}$, neglecting the higher order terms is given by [9],

$$\vec{F} = (\vec{p}\cdot\nabla)\vec{E} \qquad (1)$$

For an applied AC field, the time averaged force on a nanotube is given by [10],

$$\vec{F}_{DEP} = \Gamma \cdot \varepsilon_s \,\mathrm{Re}\{K_f\}\nabla\left|\vec{E}\right|^2 \qquad (2)$$

The factor K_f depends on the complex permittivities of both the nanotube and the dispersing solution. For a cylindrical object like the nanotubes, this factor is approximated to

$$K_f = \frac{\varepsilon_n^* - \varepsilon_s^*}{\varepsilon_s^*} \quad , \quad \varepsilon^* = \varepsilon - i\frac{\sigma}{\omega} \qquad (3)$$

where σ is the conductivity, ε is the real permittivity, and ω is the angular frequency of the applied AC field. The subscripts *n* and *s* denote the nanotube and dispersing solution respectively.

The geometrical factor Γ is given by

$$\Gamma = \frac{\pi}{6} r^2 l \qquad (4)$$

where *r* and *l* are the radius and length of the nanotube.

2.2 The FEM model

Figure 1 illustrates the geometry and boundary conditions used in the FEM model. The cylindrical nanotube is modeled in 2-D as a rectangle of length 5 μm and height of 10 nm. The micro-cantilever electrodes are modeled with a height of 4 μm, and variable spacing *d* and length *L*. A depth of 4 μm is defined for the electrodes and 10 nm for the nanotube. In the AC/DC module, the electrodes subdomain is specified as semi-insulating GaAs, the heavily n-doped upper layer boundary is specified a positive bias and negative bias on the left and right electrodes respectively. The outer boundaries of the electrolyte solution modeled as the surrounding box are defined as insulating. The continuity conditions are used for the rest of the boundaries. The module solves the Laplace equation $\nabla^2\phi = 0$ for the potential to derive the electric field. In the structural mechanics module, however, only the nanotubes subdomain is active.

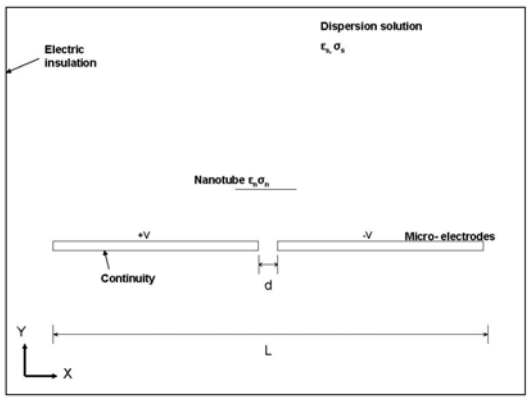


Figure 1 FEM Model definition

Due to the very high aspect ratio of the nanotubes and micro-electrodes, a combination of mapped and free meshes [11] was used to obtain an efficient FEM model as shown in Figure 2. The longer boundaries of the nanotubes were meshed by specifying 500 edge elements each.

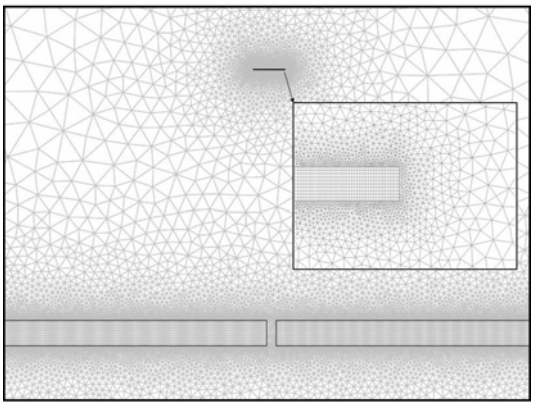


Figure 2 Mesh profile of the structure. Inset shows close-up of the nanotube tip.

2.3 Electric field and DEP force

After setting up the model as described in the previous section, the electric field is solved for around the microelectrodes in the AC/DC module. Figure 3 shows a streamline plot of the normal electric field lines in the solution domain around the microelectrodes. As only the upper boundary of the electrodes is conductive and driven with the AC signal, the electric field is much more intense in the top region. The density of the lines is proportional to the magnitude of the electric field. It is clear from the streamlines that the electric field intensity is maximum close to the electrode tips for this configuration. Also, the electric field gradient is computed over in the x and y direction by defining a subdomain expression using the diff () command. The solid arrows in Figure 3 indicate the direction of electric field gradient, which is towards the electrode tips.

Next, the DEP force components are defined as sub domain loads on the nanotubes in the structural mechanics module as the following expressions.

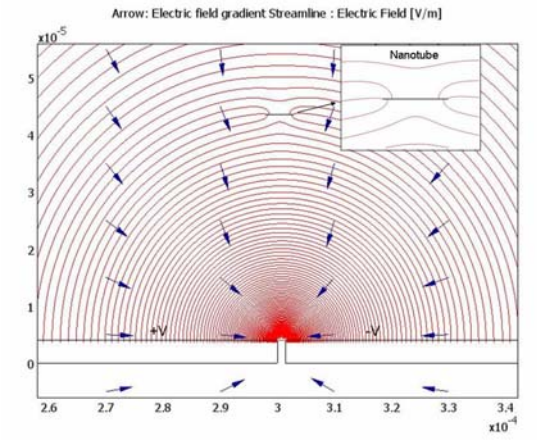


Figure 3 The electric field distribution. Streamlines show electric field and solid arrows indicate the electric field gradient (NOTE: Arrow lengths do not represent magnitude of the electric field gradient). Inset shows the electric field distorting around the nanotube.

$$F_{DEPx} = \Gamma \varepsilon_m \,\mathrm{Re}\{K_f\} \nabla_x \left| E_{norm} \right|^2 \quad (5)$$

and

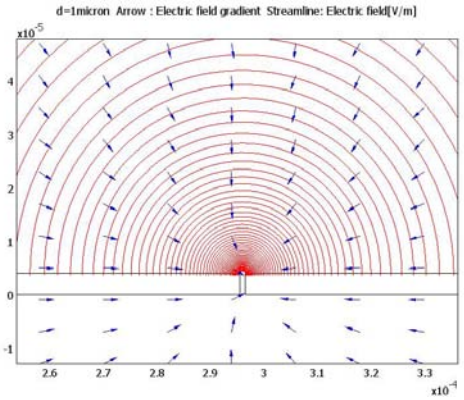
$$F_{DEPy} = \Gamma \varepsilon_m \,\mathrm{Re}\{K_f\} \nabla_y \left| E_{norm} \right|^2 \quad (6)$$

No structural constraints are defined on the nanotubes, as they are freely floating in the solution. With this model setup, the effects of various parameters on the free nanotube motion is studied and presented in the next section.

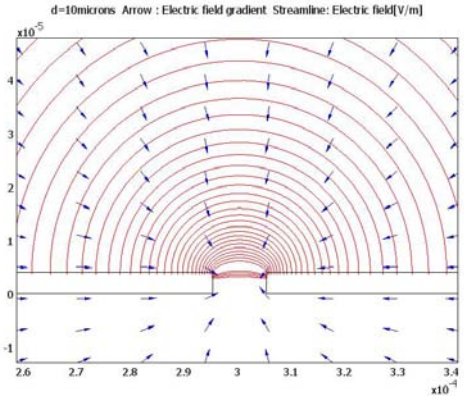
3 Results

3.1 Effect of electrodes spacing

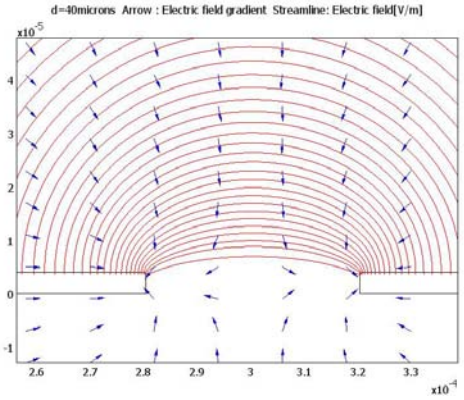
The effect electrode spacing has on the maximum electric field value, and the direction of the electric field gradient is analyzed here. The spacing is increased from 1μm to 40μm. The end to end length of the electrodes L is fixed at 200 μm here. Figure 4 shows the streamline plots of the electric fields at the tip regions for various spacings. For a short spacing of 1 μm, as shown in Figure 4(a), the electric field value has a maximum value in the order of 10^8 V/m and confined very strongly at the tips.



(a)



(b)



(c)

Figure 4 Streamline plot of electric field lines close to the electrode tips. The arrows indicate the direction of electric field gradient **(a) d=** 1µm E_{max}= 2.3E+8 V/m; **(b)** d=10 µm, E_{max} = 5.0E+7 V/m;**(c)** d= 40 µm, E_{max} = 4.8E+7 V/m

The electric field value near the outer electrode edges is of the order of 10^6 V/m. The arrows depicting the electric field gradient are all strongly directed towards the center of the two electrode tips, which is desirable for precise placement of the nanotubes. As the spacing is increased to 10 µm, the maximum intensity of the electrical field decreases by almost an order of magnitude to 10^7 V/m. Also, the directionality of the arrows towards the center of the tips is weaker, and begins diverging as shown in Figure 4(b). For a spacing of 40 µm as shown in Figure 4(c), the electric field further weakens, and the electric field gradient arrows diverge, pointing towards the two electrode tips separately. This shows that the minimum possible electrode spacing is most desirable for precise SWNTs manipulation.

3.2 Effect of bias voltage

The bias voltage in the above model is varied from 10V to 100V and its effect on the nanotubes displacement is studied, with an electrode spacing of 1 µm. Figure 5 shows a plot of applied voltage and the nanotubes displacement. The curve fit shows that the displacement increases as the square of the voltage. This behavior is expected, as the DEP force applied on the tubes as shown from Equation 2, is directly proportional to the square of the magnitude of the electric field.

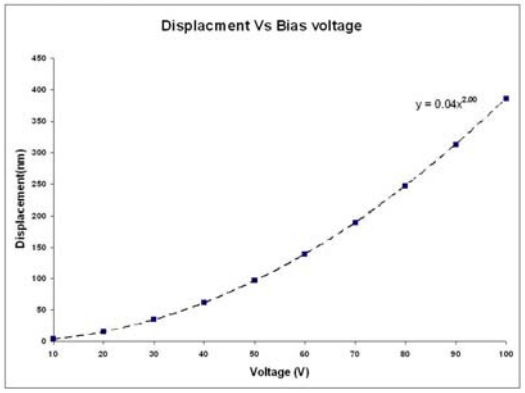


Figure 5 Simulated nanotube displacement vs bias voltage (big dots). The equation for the curve fit (dash line) is also shown.

3.3 Effect of permittivity

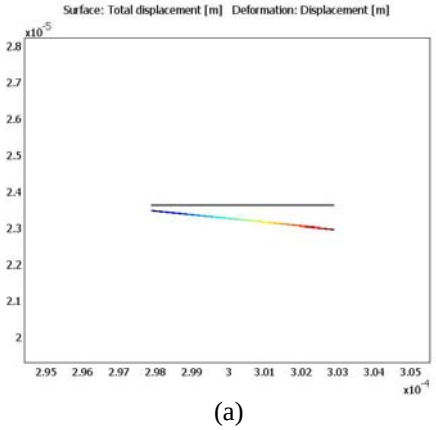
For relatively high frequencies in the order of MHz, it follows from equation (3) that,

$$\mathrm{Re}\{K_f\} = \frac{\varepsilon_p - \varepsilon_m}{\varepsilon_m} \qquad (7)$$

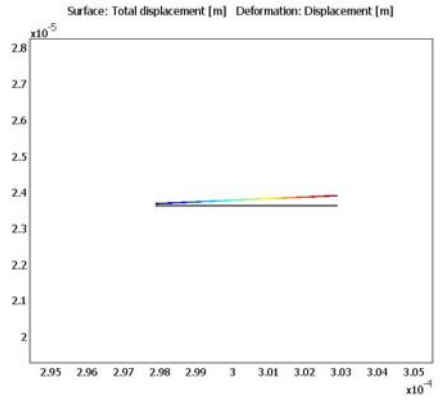
Equation (7) indicates that the direction and magnitude of the DEP force on a nanotube are strongly dependent on its relative permittivity with respect to that of the solution. If the permittivity of the nanotube is greater than that of the solution, then it moves towards the region of higher electric field, this is termed positive DEP. Similarly, if its permittivity is lower than that of the surrounding, then it moves towards region of low electric field, called negative DEP.

The relative permittivity values of semiconducting nanotubes are assumed to vary from 1 to $5\varepsilon_o$, and that of metallic nanotubes to be typically above $10\varepsilon_o$ [12]. A nanotube will be either attracted towards or repelled away from the electrodes depending on it permittivity in a properly chosen dispersion solution. This phenomenon can be used to effectively separate semiconducting nanotubes from metallic ones.

As illustrated in Figure 6(a), a metallic nanotube of permittivity $40\varepsilon_o$ dispersed in IPA of permittivity $18.6\varepsilon_o$ is seen to displace towards the electrode at a driving frequency of 2MHz. The tube thus demonstrates positive DEP. Figure 6(b) shows a semiconducting nanotube of permittivity $2.7\varepsilon_o$ dispersed in the same solution, and it is seen to bend away from the electrodes thus demonstrating negative DEP.



(a)



(b)

Figure 6 Positive and negative DEP on nanotubes. **(a)** Nanotube of higher permittivity than surrounding shows positive DEP; **(b)** Nanotube of lower permittivity than surrounding shows negative DEP. [NOTE: The horizontal bars represent the initial position of the nanotube]

The dispersion solution used thus plays a key role in determining the permittivity range of the nanotubes deposited or sorted. For instance, if a popular electrolyte like sodium dodecylsulfate (SDS) solution with a relative permittivity of $40\varepsilon_o$ is chosen, then only metallic nanotubes of permittivity value above $40\varepsilon_o$ will be deposited on the nanotubes, and the others repelled. This thus serves as a selective deposition or sorting technique. Other solutions commonly used are 2-propanol (IPA) with permittivity $18.6\varepsilon_0$, and ethanol with permittivity $40\varepsilon_0$ - $60\ \varepsilon_0$.

3.4 Effect of initial nanotubes orientation

The effect of initial placement of the nanotubes with respect to the electrodes is simulated. As in the actual experiment, nanotubes are randomly scattered around the device in all directions. The gradient of the electric field always points towards the tips of the electrode as shown earlier. This implies a net force pointing towards the tip on the nanotubes in case of the positive DEP, and hence any high aspect ratio particle like a cylindrical nanotube will tend to align along the field and then move towards the tips.

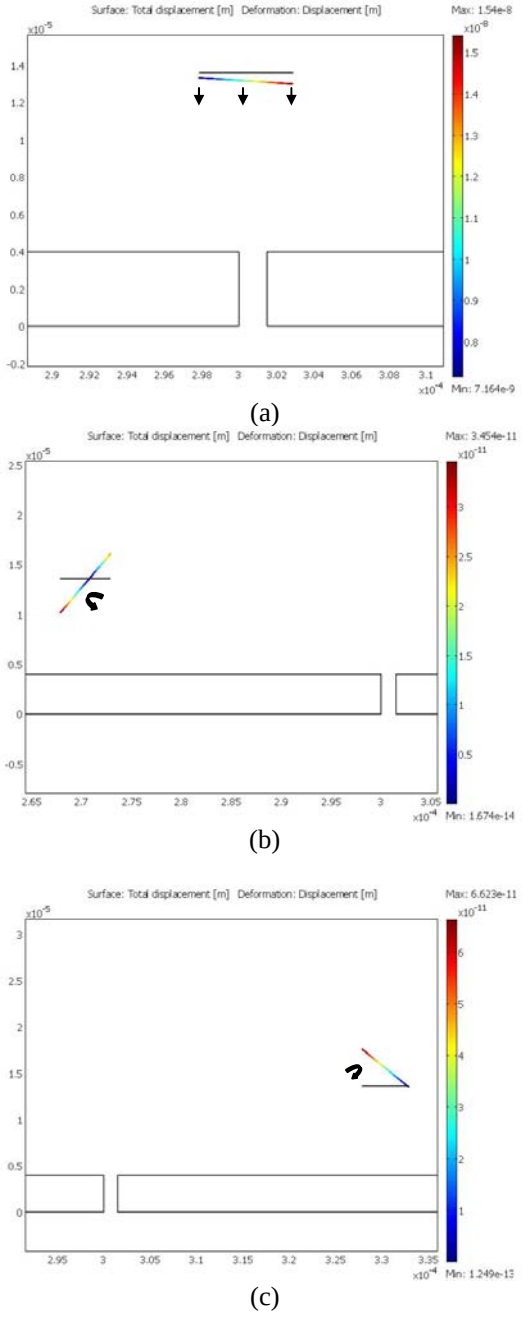


Figure 7 Effect of initial orientation on movement (a) Nanotube directly above the microelectrodes tips moving down directly; (b) Nanotube roating on the left of the tips; (c) Nanotube rotating on the right of the tips.

As shown from Figure 7(a), a nanotube placed above the electrode tips experiences minimal rotation as it is already aligned along the field, but experiences maximum displacement towards the tips. However, for a nanotube towards left or right of the tips, and away from it, the force tends to rotate the nanotube such that it is parallel to the electrical field and move it along the direction of the electric field gradient as shown in Figure 7(b) and (c) respectively.

4.0 Conclusion and future work

In conclusion, the dielectrophoresis phenomenon for nanotubes manipulation has been simulated successfully using the multi-physics features of the COMSOL package. For a further advanced model, the fluid dynamics module may be employed along with the moving mesh (ALE) feature to determine the effect of drag forces on the nanotubes dispersion. The parametric analysis done here will be used in determining the experimental parameters such as, biasing voltage, AC driving frequency, and dispersion solution to be used. With the calculated results hence, a novel micro-cantilever device will be designed and fabricated.

5. References

[1] Martel R,Schmidt T,Shea H R,Hertel T and Avouris Ph., "Single and multi-wall carbon nanotube field-effect transistors", *Appl. Phys. Lett.* **Vol.73**, pp. 2447-9 (1998).

[2] Z Yao,C.L. Kane, C.Dekker, "High-field Electrical Transport in Single-Wall Carbon Nanotubes" *Phys. Rev. Lett.*,**Vol.84,** pp.2941-4(2000).

[3] Hertel T,Martel R and Avouris, "Manipulation of individual carbon nanotubes and their interaction with surfaces", *J. Phys. Chem. B*, **Vol.102**, pp. 910-5 (1998).

[4] Huang Y,Duan X,Wei Q and Lieber C M, " Directed assembly of One-dimensional Nanostructures into Functional Networks", *Science*, **Vol. 291**, pp. 630-3 (2001).

[5] Dimaki and Boggild, "Dielectrophoresis of carbon nanotubes using microelectrodes: a numberical study",*Nanotechnology*,**Vol. 15**, pp. 1095-1102 (2004).

[6] Nagahara,Amlani,Lewenstein,Tsui, "Directed placement of suspended carbon nanotubes for nanometer-scale assembly", *Appl. Phys. Lett.*, **Vol. 80**, pp 3826-8 (2002).

[7] V.Mathur, J.Li and W.D.Goodhue, **"**FEM simulation of a micro-cantilever optical-MEMS sensor**"** *Proceedings of the Comsol Users Conference, Boston 2006*, pp 333-8 (2006).
[8] Green, Ramos and Morgan, "Ac electrokinetic : a survey of sub-micrometer particle dynamics",*J.Phys.D:Appl. Phys*., **Vol. 33**,pp. 632-641(2000).
[9]. Wangsness, *Electromagnetic Fields*, pp.128-9,J Wiley and Sons, 2nd Edition (1986)
[10]Asokan,Jawerth,Carroll,Cheney,Washburn,Superfine, "Two dimensional manipulation and orientation of Actin-Myosin systems with dielectrophoresis", *Nano Lett.*,**Vol.3** ,pp.431-437 (2003)
[11] "Comsol new features guide", **Version 3.3**, pp. 58-74.
[12] Grimes,Dickey,Mungle,Ong and Qian, "Effect of purification of the electrical conductivity and complex permittivity of multiwall carbon nanotubes",**Vol.90**,No.8,pp. 4134-7(2001).