Simulation Study on Trajectory of Dielectrophoretic Force Controlled Nanowires

Quan Tao, and Guangyong Li
Department of Electrical and Computer Engineering
University of Pittsburgh, Pittsburgh, PA

***Abstract* — Nanoscale manipulation is of tremendous importance in the application of nanowire-based devices like chemical and biological sensors, light-emitting diodes, and field effect transistors. In order to fabricate nanodevices with high throughput, nanowires need to be manipulated towards pre-defined electrodes with high efficiency. Dielectrophoresis (DEP) provides a noninvasive, nondestructive method to effectively align nanowires. In this paper, the trajectory of single nanowire manipulated by DEP force in liquid is analyzed and simulated. Because the electrode gap is usually shorter than the nanowire, the electric field generated by the electrode pair is highly nonuniform along the nanowire. Using an approach similar to finite element, the DEP force applied to the nanowire as well as the torque induced by DEP can be precisely calculated by dividing the nanowire into small segments. By assuming the electric field is uniform along each segment, the total force and torque on the nanowire induced by DEP can be obtained. By considering the drag force from the surrounding liquid, the overall force on the nanowire is calculated, thus the trajectory of nanowire manipulated by DEP force is obtained. The simulation results show that the DEP force is able to attract the nanowire to electrodes and to force it bridge the gap between electrodes.**

Index Terms – Dielectrophoresis, Hydrodynamics, Nanowires, Nanomanipulation

I. INTRODUCTION

Since Pohl's pioneering contributions on dielectrophoresis (DEP) [1], many researchers have performed extensive investigation on nanoscale manipulation using dielectrophoretic forces [2, 3]. For example, nanowires can be assembled in a variety of device applications like field effect transistors, light-emitting diodes, and biological sensors [4, 5]. Specially, by introducing a non-uniform electric field, DEP force is able to align nanowires to pre-defined electrodes, therefore constructing desired electronic devices. S. Raychaudhuri *et al* experimentally demonstrated that InAs nanowires can be aligned from solution to intricate electrodes with high efficiency [2]. E. M. Freer *et al* showed simultaneous high-yield assembly of large numbers of single nanowires to electrodes array [3]. In order to precisely assemble the nanowires, a comprehensive study on the nanowire trajectory is imperative. Although significant progress has been made in experimentally aligning nanowires to build electronic devices, theoretical analysis and simulation study on the trajectory of single nanowire is still absent.

Affected by the non-uniform electric field and the surrounding fluid, the translational motion of single nanowire is controlled by DEP force and hydrodynamic drag force. The DEP force depends on the geometry of the nanowire, electrical property of the nanowire and the surrounding medium, the position and the orientation of the nanowire in the non-uniform electric field. On the other hand, the drag force is related to the geometry and velocity of the nanowire as well as the viscosity of the fluid. In addition, besides the translational movement, the motion of single nanowire also involves rotation in the fluid because of DEP torque and drag toque, which increases the complexity in the theoretical analysis.

In this paper, we proposed a theoretical model to calculate forces and torques on the nanowire. The trajectory of single nanowire is estimated through the simulation study. Our simulation study can clearly demonstrate that the nanowire is attracted to and bridge the pre-defined electrodes using DEP force.

II. MODELING

DEP force is generated because of the interaction between the non-uniform electric field and the induced effective dipole of the particle. For a nanowire with radius r and length L, its effective polarisability depends on the orientation of the nanowire. In previous work [6], we combined Morgan [7] and Pohl's [8] work and derived the DEP force equation when the electric field has an angle θ with the nanowire,

$$\boldsymbol{F}_{DEP} = \frac{1}{6}\pi r^2 \varepsilon_m L \nabla \boldsymbol{E}^2 \left[cos^2\theta Re\left\{\frac{\tilde{\varepsilon}_p - \tilde{\varepsilon}_m}{\tilde{\varepsilon}_m}\right\} + 2sin^2\theta Re\left\{\frac{\tilde{\varepsilon}_p - \tilde{\varepsilon}_m}{\tilde{\varepsilon}_p + \tilde{\varepsilon}_m}\right\}\right], \quad (1)$$

where $\boldsymbol{E}$ is the electric field, ε_m and ε_p are the permittivities of the medium and the nanowire, and $\tilde{\varepsilon}_m$ and $\tilde{\varepsilon}_p$ are the complex permittivities of the medium and the nanowire, respectively. The complex permittvity $\tilde{\varepsilon}$ is defined as $\tilde{\varepsilon} = \varepsilon - i\frac{\sigma}{\omega}$, where σ is the electric conductivity, and ω is the angular frequency of the electric field. Equation (1) is limited to the situation when the scale of field nonuniformity is larger than the dimension of the nanowire. However, since the length of the nanowire is comparable to the gap between the microelectrodes, the non-uniformity of the electric field around the nanowire is unavoidable. To address this issue, we divided the whole nanowire to a couple of small cylinders, as shown in Fig. 1, such that the electric field around each small cylinder is treated as uniform. Each segment is polarized to yield an effective dipole which interacts with the electric field and generates an individual DEP force. The composition of these DEP forces on each cylinder provides the net DEP force on the whole nanowire. Moreover, the DEP forces on each cylinder generate torques with respect to the center of mass of the nanowire.

The DEP torque that an electric field exerts on a dipole is given by

$$T = \boldsymbol{p} \times \boldsymbol{E}, \quad (2)$$

where $\boldsymbol{p}$ is the induced dipole moment. For a lossy dielectric particle in an AC electric field, the DEP torque is frequency-dependent and tends to align the effective dipole with the direction of the electric field [9]. As shown in Fig. 1, the torque on each effective dipole depends on the local electric field and can be expressed as

$$T_{DEPi} = \frac{1}{3}\pi r^2 l \varepsilon_m (L_\perp - L_\parallel) E_{i\parallel} E_{i\perp} Re[\boldsymbol{K}_\parallel \boldsymbol{K}_\perp], \quad (3)$$

where for prolate nanowires, the depolarization factors $L_\perp = \frac{1}{2}$, $L_\parallel = 0$, $E_{i\parallel}$ and $E_{i\perp}$ are parallel and perpendicular components of the local electric field, respectively, and the complex polarization factors are defined as

$$\boldsymbol{K}_\perp = \frac{\tilde{\varepsilon}_p - \tilde{\varepsilon}_m}{3[\tilde{\varepsilon}_m + (\tilde{\varepsilon}_p - \tilde{\varepsilon}_m)L_\perp]} \qquad \boldsymbol{K}_\parallel = \frac{\tilde{\varepsilon}_p - \tilde{\varepsilon}_m}{3[\tilde{\varepsilon}_m + (\tilde{\varepsilon}_p - \tilde{\varepsilon}_m)L_\parallel]}. \quad (4)$$

The sum of the DEP torques on each segment yields the total DEP torque on the nanowire.

The motion of the nanowire is also affected by hydrodynamic drag force and drag torque. For a prolate cylinder moving in the fluid, the drag force depends on the velocity and moving direction of the nanowire [10]. Mathematically,

$$\boldsymbol{F}_{DRAG\parallel} = -\frac{2\pi\eta L}{\ln\left(\frac{L}{r}\right) - 0.5}\boldsymbol{v} \quad (5) \qquad \boldsymbol{F}_{DRAG\perp} = -\frac{4\pi\eta L}{ln\left(\frac{L}{r}\right) + 0.5}\boldsymbol{v} \quad (6)$$

where $\boldsymbol{F}_{DRAG\parallel}$ and $\boldsymbol{F}_{DRAG\perp}$ are the drag force when the nanowire is moving parallel to and perpendicular to its axis, respectively, η is the viscosity of the fluid, and $\boldsymbol{v}$ is the velocity of the nanowire. For a nanowire moving at arbitrary direction, we can orthogonally decompose the velocity $\boldsymbol{v}$, shown in Fig. 2(a). Therefore, the drag force can be calculated as

$$\boldsymbol{F}_{DRAG} = -\frac{2\pi\eta L}{\ln\left(\frac{L}{r}\right) - 0.5}\boldsymbol{v}_\parallel - \frac{4\pi\eta L}{ln\left(\frac{L}{r}\right) + 0.5}\boldsymbol{v}_\perp \quad (7)$$

To calculate the drag torque on a nanowire, the whole nanowire is evenly divided to N segments of small cylinders [11], shown in Fig. 2(b). As the nanowire rotates with an angular velocity of ω in the medium, each segment receives a drag force $\boldsymbol{F}_{DRAGi}$ depends on its velocity $\boldsymbol{v}_i$. The drag force on each cylinder introduces a torque with respect to the center of mass of the nanowire. The total drag torque is estimated by summing up the drag toques from each segment.

$$T_{DRAG} = -2\sum_{i=1}^{\frac{N}{2}} \frac{\frac{4\pi\eta L}{N}}{\ln\left(\frac{L}{Nr}\right) + 0.5}\omega\left[\left(i - \frac{1}{2}\right)\frac{L}{N}\right]^2 = -\frac{(N^3 - N)\pi\eta L^3\omega}{3N^3\left[\ln\left(\frac{L}{Nr}\right) + 0.5\right]} \quad (8)$$

III. Simulation and Results

Based on the derived model on different forces and torques, a comprehensive simulation study on the trajectory of single nanowire can be implemented, shown in Fig. 3. We utilized Ansoft Maxwell software to simulate the distribution of a non-uniform electric field. The DEP force and torque are able to be calculated based on the position and orientation of the nanowire in the non-uniform electric field. At each step, the drag force and torque can be obtained according to the current translational velocity and rotational angular velocity. The net force and torque are able to provide the acceleration and angular acceleration for current

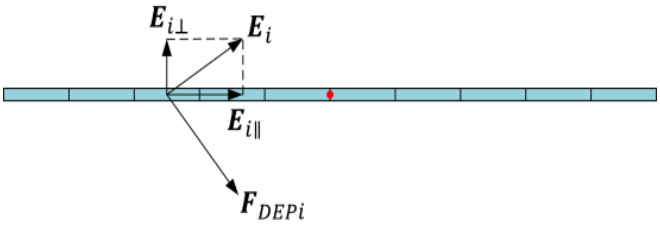

Fig. 1 Evenly divide the nanowire to calculate the DEP force and the DEP torque.

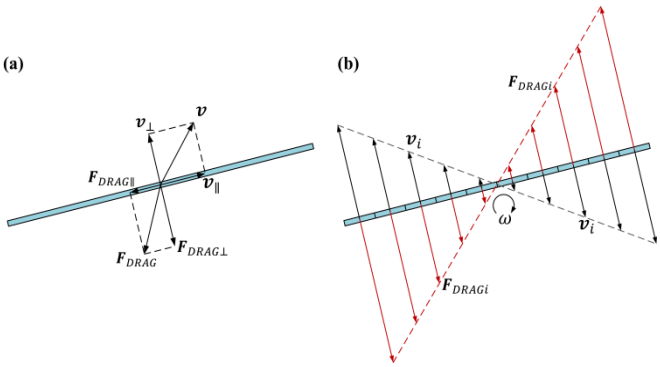

Fig. 2(a) Orthogonally decompose the velocity to calculate the drag force. (b) Evenly divide the nanowire to obtain the total drag torque.

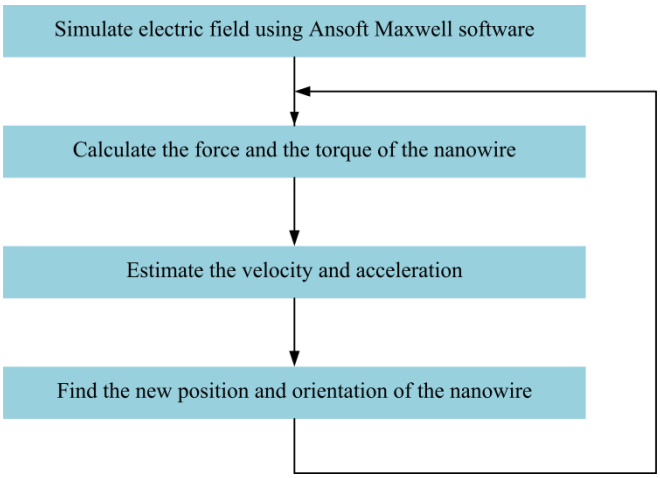

Fig. 3 A flow chart of the simulation

step. We assume the nanowire will move according to the calculated acceleration and angular acceleration during very small time duration. As the nanowire reaches a new position, the new forces, torques, velocity, and angular velocity can be calculated using the same approach. Hence the trajectory of the nanowire can be simulated iteratively.

A pair of sharp electrode with length 100μm and width 1μm is constructed in Ansoft Maxwell software. The gap between the electrodes is 5μm. A non-uniform electric field was created by applying an AC voltage excitation with amplitude ±5V and frequency 1MHz, shown in Fig. 4. Both the electric field $\boldsymbol{E}$ and the gradient form $\nabla\boldsymbol{E}^2$ have larger values near the gap of electrodes. According to Equations (1) and (3), $\boldsymbol{E}$ and $\nabla\boldsymbol{E}^2$ determine the DEP torque and the DEP force, respectively, therefore affecting the motion of the nanowire. We simulated the trajectory of single zinc oxide (ZnO) nanowire with length 10μm and radius 30nm. Since ZnO nanowire will degrade in water, organic

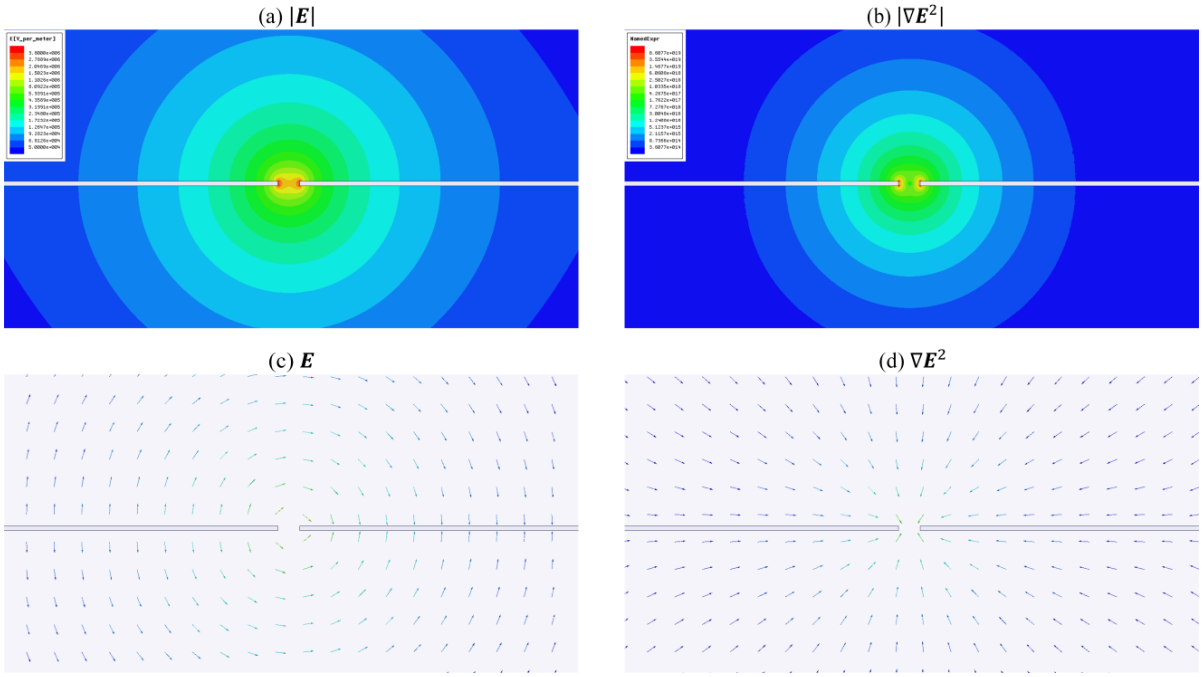

Fig. 4 (a) The magnitude of the electric field $\boldsymbol{E}$. (b) The magnitude of the gradient form $\nabla \boldsymbol{E}^2$. (c) The vector plot of the electric field $\boldsymbol{E}$. (d) The vector plot of the gradient form $\nabla \boldsymbol{E}^2$.

solvents (isopropanol) are used as the suspending medium. Based on the simulated electric field and the parameters of the nanowire and the medium, a typical DEP force on a nanowire near the electrodes is at the order of several pico-newtons, which is adequate to overcome the Brownian motion of the nanowire. Because of the symmetric distribution of the electric field, we consider the initial position of the center of nanowire is at $(10\mu m, 15\mu m)$ with the long axis of the nanowire parallel to the electrodes. The initial velocity and angular velocity are zero. The trajectory of the nanowire is plotted in Fig. 5. Because the polarisability of ZnO nanowire is greater than the surrounding isopropanol at $1MHz$, the nanowire receives positive (attractive) DEP force and is driven towards strong electric field region. Since the DEP force is proportional to $\nabla \boldsymbol{E}^2$**,** the nanowire translates to the gap of electrodes along the direction of $\nabla \boldsymbol{E}^2$. Moreover, the non-uniform electric field exerts DEP torques on the nanowire to align it with the electric field $\boldsymbol{E}$. The nanowire receives stronger DEP force and DEP torque when it moves closer to the gap of electrodes, therefore translating and rotating faster gradually. At time 2.79s**,** the nanowire hits the electrode and will be stuck due to the strong Van der Waals force. Hence the nanowire will only rotate around the connection point without any translational motion during later time steps. The conservation of kinetic energy enables us to estimate the instant angular velocity when the nanowire hits the electrode,

$$\frac{1}{2}m|\boldsymbol{v}|^2 + \frac{1}{2}I\omega^2 = \frac{1}{2}I_{new}\omega_{new}^2 \qquad (9)$$

where m and I are the mass and moment of inertia of the nanowire, I_{new} and ω_{new} are the new moment of inertia and new angular velocity of the nanowire after it hits the

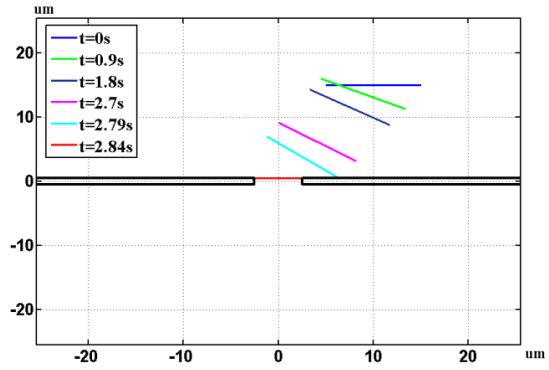

Fig. 5 Trajectory of single nanowire at different time.

electrodes, respectively. Similar to previous simulation, the DEP and drag torque, the angular velocity, the angular acceleration, and the new position can be estimated during each iteration. The nanowire will rotate in the counterclockwise direction and bridge the electrodes ultimately.

IV. Conclusion

Precise manipulation of nanowires is extremely important in the application of nanowire-based devices. Applying an AC excitation across pre-defined electrodes, a non-uniform electric field is generated in space. The interaction between the non-uniform electric field and the induced effective dipole exerts DEP force and DEP torque on a nanowire, therefore controlling its motion. Moreover, the movement of the nanowire in fluid is affected by hydrodynamic drag force and drag torque. In this paper, we proposed a comprehensive model to estimate DEP force, DEP torque, drag force, and drag torque that the

nanowire receives. Ansoft Maxwell software is utilized to simulate the non-uniform electric field produced by a pair of sharp microelectrodes. We also simulated the trajectories of a nanowire close to the electrodes. The result indicates that the nanowire will be attracted towards and bridge the electrodes, which provided simulation support for DEP manipulation.

ACKNOWLEDGEMENT

This research is supported by NSF grant CNS 1035563.

REFERENCES

[1] H. A. Pohl, Dielectrophoresis. London: Cambridge University Press, 1978.
[2] S. Raychaudhuri, et al., "Precise Semiconductor Nanowire Placement Through Dielectrophoresis," Nano Letters, vol. 9, pp. 2260-2266, Jun 2009.
[3] E. M. Freer, et al., "High-yield self-limiting single-nanowire assembly with dielectrophoresis," Nature Nanotechnology, vol. 5, pp. 525-530, Jul 2010.
[4] S. A. Dayeh, et al., "High electron mobility InAs nanowire field-effect transistors," Small, vol. 3, pp. 326-332, Feb 2007.
[5] C. P. T. Svensson, et al., "Monolithic GaAs/InGaP nanowire light emitting diodes on silicon," Nanotechnology, vol. 19, Jul 30 2008.
[6] G. L. Quan Tao, and Liming Liu, "Selective Manipulation of ZnO Nanowires by Controlled Dielectrophoretic Force," presented at the IEEE NANO 2011, Portland, 2011.
[7] H. Morgan, and G. G. Green, AC Electrokinetics: colloids and nanoparticles: Research Studies Press Ltd., 2003.
[8] H. A. Pohl, "Dielectrophoretic force: a comparison of theory and experiment," Physical Biological Science, vol. 6, p. 27, 1978.
[9] T. B. Jones, Electromechanics of Particles: Cambridge University Press, 1995.
[10] H. C. Berg, Random Walks in Biology: Pricention University Press, 1993.
[11] K. Keshoju, et al., "Magnetic field driven nanowire rotation in suspension," Applied Physics Letters, vol. 91, Sep 17 2007.