# Electrokinetic assembly and manipulation I

**Lecture by Liu, Wing Kam**

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## Outline

- Introduction of electric field guided assembly
- IEFEM: Coupled electrokinetics and hydrodynamics
- IEFEM simulation; nanowire assembly
- IEFEM simulation; one dimensional assembly
- IEFEM simulation; biomaterial manipulation

• **Introduction of**
• **electric field guided assembly**

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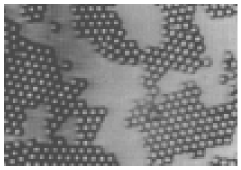
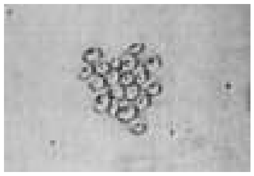
## E-field assembly of micro-particles

•Massive assembly by electric field

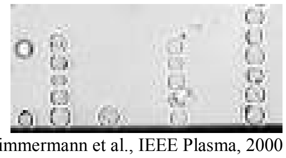
-Colloidal crystals assembly


Trau et al., Langmuir,2003

-Self assembly & two dimensional patterning of cell arrays by electrophoretic deposition


Brisson and Tilton, Biotech and Bioeng., 2002

-Precise assembly and electro-deformation of cells


Zimmermann et al., IEEE Plasma, 2000

• Advantages
-Massive particles, precise, reproducible process

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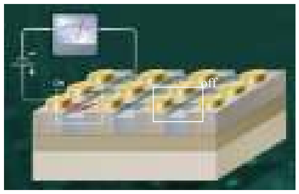
## Nanomanufacturing of electronic/molecular devices

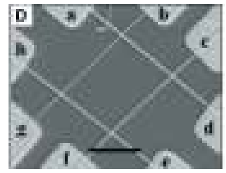
Carbon Nanotube Based Memory Devices



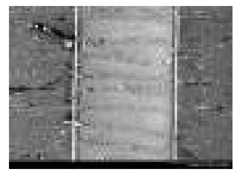
*Source: http://www.nantero.com/nram.html*

Rueckes et al., Science, 2000

Carbon Nanotube Assembly Method



Cross-bar array of Si NWs by fluid flow
Y. Huang et al., Science, 2001



Electric field guided assembly of NWs
J. Chung, U. Washington

**Challenge:** A production chip requires millions of these CNTs to be assembled precisely between the micro/nano electrodes

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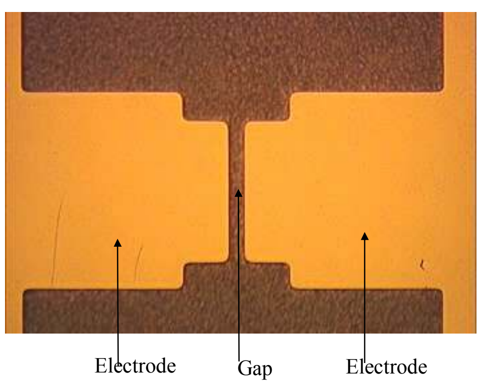
## Nanowire assembly by an AC field




(5 MHz, 0.5v/µm)

•Design parameters

electrode geometry, e-field strength, and gap size compatible with nanowires

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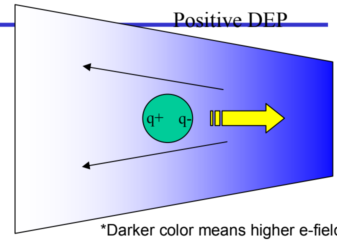
# Dielectrophoresis (DEP)

• The force exerted by an electric field (**E**) on dipole moment p:

$$\mathbf{F} = (\mathbf{p} \cdot \nabla)\mathbf{E}$$

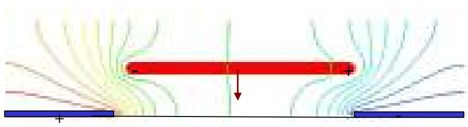



*Darker color means higher e-field.

• In AC field, Effective Dipole Moment (EDM) theory gives DEP force:

$$\boxed{\mathbf{F}_{\mathrm{DEP}} = \Gamma \cdot \varepsilon_{\mathrm{m}} \operatorname{Re}\{K_{\mathrm{f}}\} \nabla |\mathbf{E}|^2}$$ (Jones, T. B. *Electromechanics of particles*, 1995)

Geometrical factor $\Gamma = 2\pi a^3$, Polarization $K_f = (\varepsilon_m^* - \varepsilon_p^*)/(\varepsilon_m^* + 2\varepsilon_p^*)$, ε is the permitivity of media and particle



NOT applicable for Particle assembly modeling

• Particle size is large compared to gap size
• Local electric field distortion is essential

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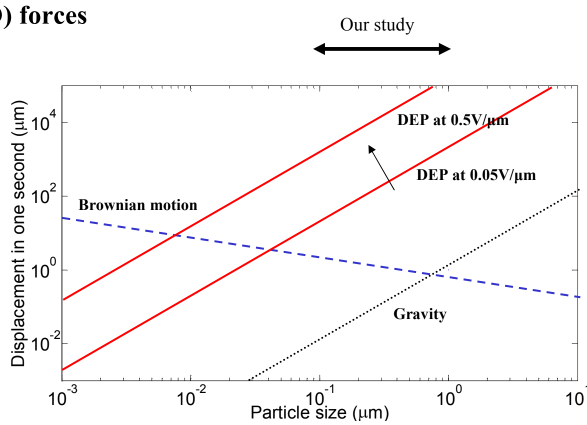
# Forces in electromechanical problems

**Electrohydrodynamic (EHD) forces**

- Drag force induced by flow (including electroosmotic flow)
- Electrophoretic force (EP)
- Dielectrophoresis (DEP) force
- Other factors playing minor roles
  - Brownian motion
  - Temperature change due to E field




Spherical particle 10μm above two planar electrodes with a spacing of 20 μm, density=1g cm$^{-3}$, viscosity=0.78Pa·s

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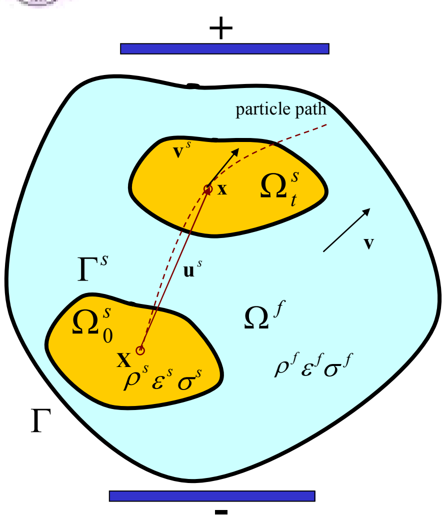
# IEFEM: Coupled electrokinetics and hydrodynamics



## Configuration of the problem




- Domain description
  - Compressible Navier-Stokes Fluid $\Omega^f$
  - Elastic Solid $\Omega^s$
  - Fluid-Solid Interface $\Gamma^s$
- Primary variables
  - Electric field $\mathbf{E}$
  - Velocity $\begin{cases} \text{solid} & \mathbf{v}^s \quad \text{in } \Omega^s \\ \text{fluid} & \mathbf{v}^f \quad \text{in } \Omega^f \end{cases}$
  - Pressure $p^f$ in $\Omega^f$
- Major charge carriers
  - Inherent charge carriers, i.e., electrons
  - Ions in fluid

## Continuum Electro-mechanics

**Maxwell equations**

$$\nabla\cdot(\varepsilon\mathbf{E}) = \rho_f$$

$$\frac{D\rho_f}{Dt} + \nabla\cdot(\sigma\mathbf{E}) = 0$$

$$\mathbf{E} = -\nabla\phi$$

$\sigma$: conductivity
$\phi$: electric potentail
$\rho_f$: free charge density

Standard BC: $\phi = \phi_0$, $-\sigma\nabla\phi\cdot\mathrm{n} = 0$,

Jump BC at interface:

$$\mathbf{n}\cdot[\![\varepsilon\mathbf{E}]\!] = \gamma_f \qquad \mathbf{n}\cdot[\![\sigma\mathbf{E}]\!] = \frac{\partial\gamma_f}{\partial t}$$

- Major charge carriers: inherent carriers

For an AC field, $\tilde{\phi}(\mathbf{x},t) = \phi^M(\mathbf{x})e^{j\omega t}$, $\quad$ $\omega$: frequency

-particle motion time scale >> 1/f : $\frac{D\rho_f}{Dt} \approx \frac{\partial\rho_f}{\partial t} = j\omega\rho_f$

Reduced Maxwell equation in complex form

$$\nabla\cdot(\tilde{\varepsilon}^f\nabla\tilde{\phi}^f) = 0, \qquad \text{in } \Omega^{\mathrm{f}},$$

$$\nabla\cdot(\tilde{\varepsilon}^s\nabla\tilde{\phi}^s) = 0, \qquad \text{in } \Omega^{\mathrm{s}},$$

$$\tilde{\varepsilon}^s\tilde{\mathbf{E}}^s\cdot\mathbf{n} = \tilde{\varepsilon}^f\tilde{\mathbf{E}}^f\cdot\mathbf{n}, \quad \text{on } \Gamma^s$$

Where $\tilde{\varepsilon} = \varepsilon + (\sigma/j\omega)$ :complex permittivity

- Major charge carriers: ions in fluid
  - Ions are external source of free charge
  - Solids are insulators

Maxwell equation + Species equation

$$\rho_f = \sum_k ez^k n^k, \ \text{in } \Omega^{\mathrm{f}}, \qquad k = 1,\ldots,N$$

$$\frac{\partial n^k}{\partial t} + \mathbf{v}^f\cdot\nabla n^k = \nabla\cdot[-\omega^k ez^k n^k\mathbf{E} + \omega^k k_B T\nabla n^k], \text{ in } \Omega^{\mathrm{f}}$$

$$n^k = 0, \qquad \text{in } \Omega^{\mathrm{s}},$$

$$\varepsilon^f\mathbf{E}^f\cdot\mathbf{n} = \varepsilon^s\mathbf{E}^s\cdot\mathbf{n}, \quad \text{on } \Gamma^s$$

$n^k$ :concentration of k$^{\text{th}}$ species, $\omega^k$ :mobility

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## Immersed formulation of IEFEM

- Augmented fluid momentum equation

$$\rho^{\mathrm{f}}\,\dot{\mathbf{v}} = \nabla\cdot\boldsymbol{\sigma} + \rho^{\mathrm{f}}\mathbf{g} + \boldsymbol{\sigma}^M + \mathcal{F}, \qquad \text{in } \Omega = \Omega^f\cup\Omega^s\cup\Gamma$$

$$\boxed{\mathcal{F} = \begin{cases}(\rho^f-\rho^s)(\dot{\mathbf{v}}^s-\mathbf{g}) + \nabla\cdot(\boldsymbol{\sigma}^s-\boldsymbol{\sigma}^f+\boldsymbol{\sigma}^M), & \text{in } \Omega^s\\ 0, & \text{in } \Omega^f\end{cases}}$$

Maxwell stress tensor

$$\boldsymbol{\sigma}^{\mathrm{M}} = \frac{1}{4}\mathrm{Re}(\underset{\sim}{\varepsilon})((\tilde{\mathbf{E}}\tilde{\mathbf{E}}^* + \tilde{\mathbf{E}}^*\tilde{\mathbf{E}}) - |\tilde{\mathbf{E}}|^2\,\mathbf{I})$$

- Augmented electric field equation
  - Inherent charge carriers

$$\nabla\cdot(\tilde{\varepsilon}^f\nabla\tilde{\phi}) + Q = 0, \qquad \text{in } \Omega, \qquad Q = \begin{cases}\nabla\cdot((\tilde{\varepsilon}^s-\tilde{\varepsilon}^f)\nabla\tilde{\phi}^s), & \text{in } \Omega^{\mathrm{s}}\\ 0, & \text{in } \Omega\setminus\Omega^{\mathrm{s}}\end{cases}$$

  - Ions

$$\nabla\cdot(\varepsilon_f\nabla\phi) + S = 0, \qquad \text{in } \Omega. \qquad S = \begin{cases}\nabla\cdot((\varepsilon_s-\varepsilon_f)\nabla\phi^s), & \text{in } \Omega^{\mathrm{s}}\\ -\rho_f, & \text{in } \Omega^{\mathrm{f}}\end{cases}$$

$$\rho_f = \sum_k ez^k n^k, \qquad \text{in } \Omega^{\mathrm{f}},$$

$$\frac{Dn^k}{Dt} = \nabla\cdot[-\omega^k ez^k n^k\mathbf{E} + \omega^k k_B T\nabla n^k] + N, \ \text{in } \Omega, \qquad N = \begin{cases}\lambda, & \text{in } \Omega^{\mathrm{s}}\\ 0, & \text{in } \Omega\setminus\Omega^{\mathrm{s}}\end{cases}$$

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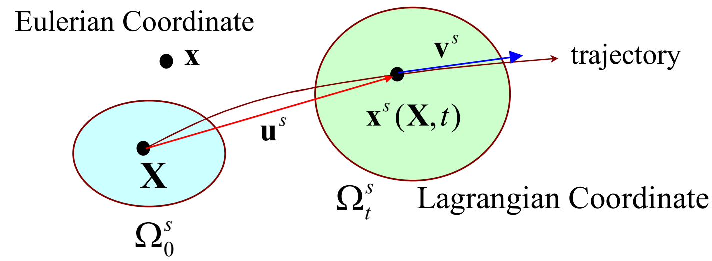
# Eulerian-to-Lagrangian (E-L) Mapping




$$(L_{\Omega_t^s}\boxed{\psi})(\mathbf{X},t) \equiv \psi(\mathbf{x}(\mathbf{X},t),t), \qquad \forall \mathbf{X} \in \Omega_0^s$$

Eulerian function    Lagrangian function

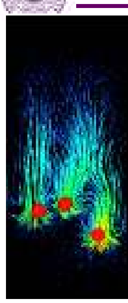
$$\dot{\psi} = \frac{\partial}{\partial t} L_{\Omega_t^s}\psi,$$

$$\nabla_{\mathbf{x}}\psi = \nabla_{\mathbf{X}} L_{\Omega_t^s}\psi \left[\frac{\partial \mathbf{x}}{\partial \mathbf{X}}\right]^{-1}$$

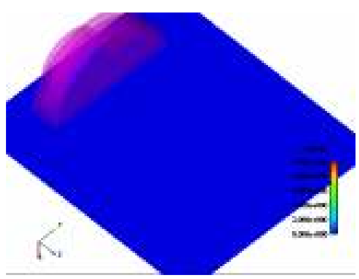
- Mapping function
  - FEM shape function
  - RKPM Dirac delta function



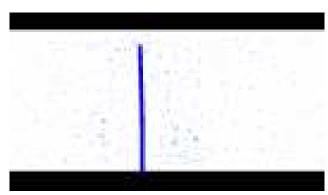
# What can the IEFEM do?



Particulate flow

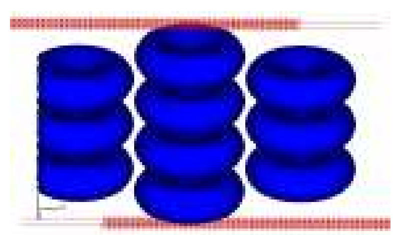


Air bag expansion



Artificial valve

RBCs in capillary

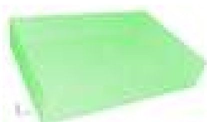


Shear of RBCs cluster

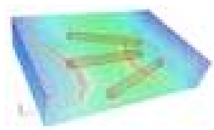
## What can the IEFEM do? (cont'd)

**Coupling of e-field with fluid-structure interaction problems**

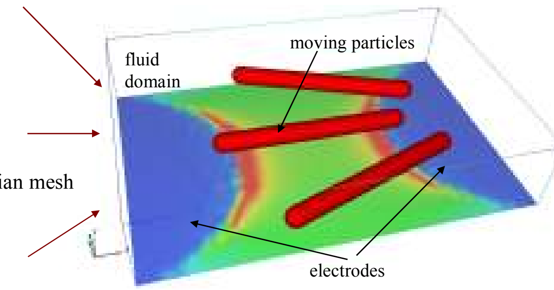
(a) Particle, Lagrangian mesh



(b) Fluid domain, Navier-Stocks flow, Eulerian mesh



(c) Electric field, Eulerian mesh with particle domains tracked separately (electric properties different from the fluid are assigned for domains occupied by particles)




(d) Coupled electrohydrodynamic modeling of the assembly of suspended particles between micro-electrodes

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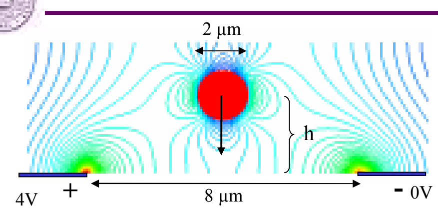
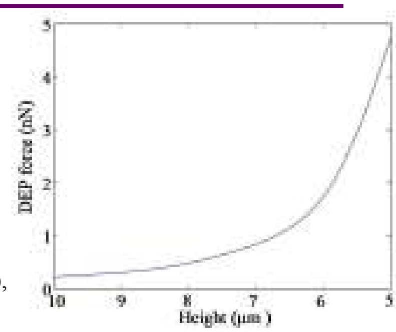
## Numerical solution vs. Effective Dipole Theory




E-field contour

Effective Dipole theory: $\langle \mathbf{F}_{\mathrm{DEP}} \rangle = \Gamma \cdot \varepsilon^f \,\mathrm{Re}\{K_f\} \nabla (E^2),$

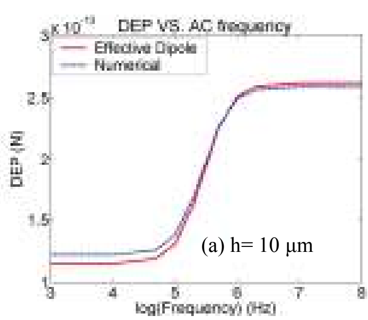


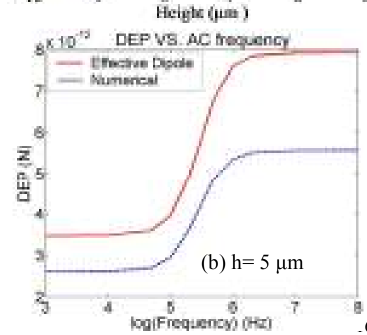

$\varepsilon^f = 20\varepsilon_0$

$\varepsilon^s = 100\varepsilon_0$

$\sigma^f = 0.0056$ s/m

$\sigma^s = 0.0112$ s/m

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**IEFEM simulation;**
**Nanowire assembly**

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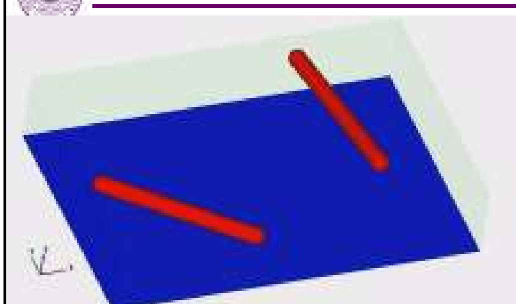
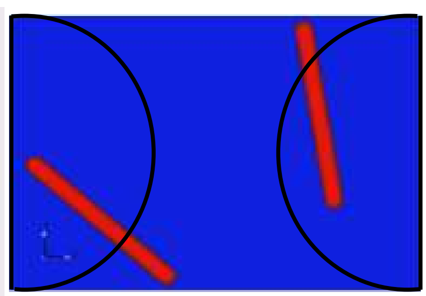
## 3D Nanowire assembly simulation



3D view



Top view

Two steps are involved in the assembly process of NWs between semi-circular shaped electrodes

- Attraction induced by DEP force
- Alignment induce by DEP torque

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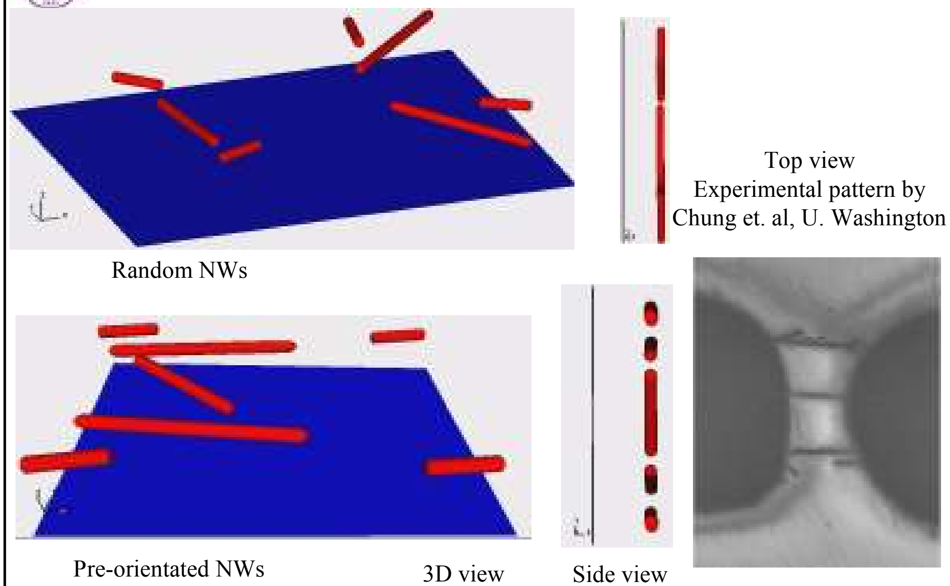
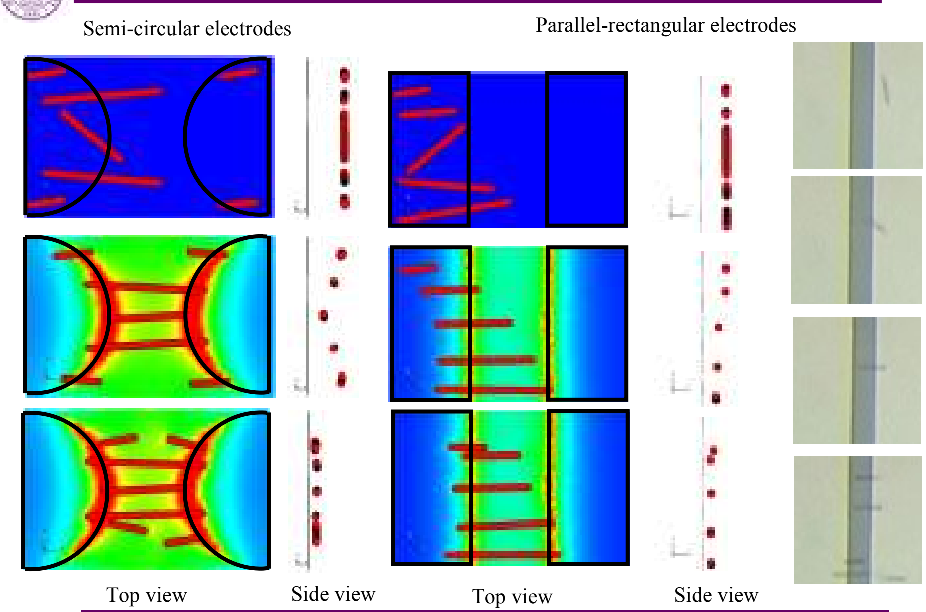
## NWs assembly between semi-circular shaped electrodes



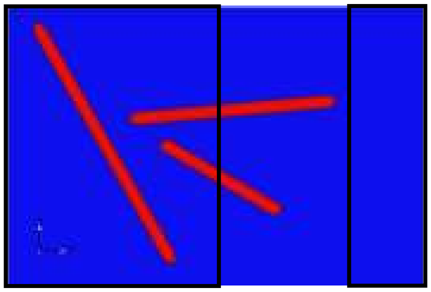


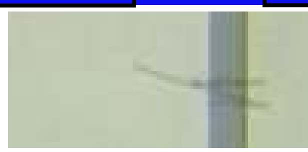

## NWs assembly patterns

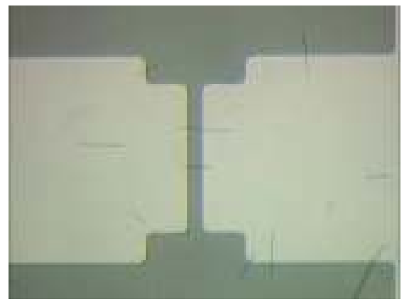


## NW assembly between rectangular shaped electrodes

When two NWs deposit close to each other, a third NW with a longer length may be deposited to connect the opposite two ends of the deposited NWs---because a high e-field region is created at the ends of the deposited NWs.
To avoid: transport and pre-orient by fluid flow







Top view
Experimental pattern by
Chung et. al

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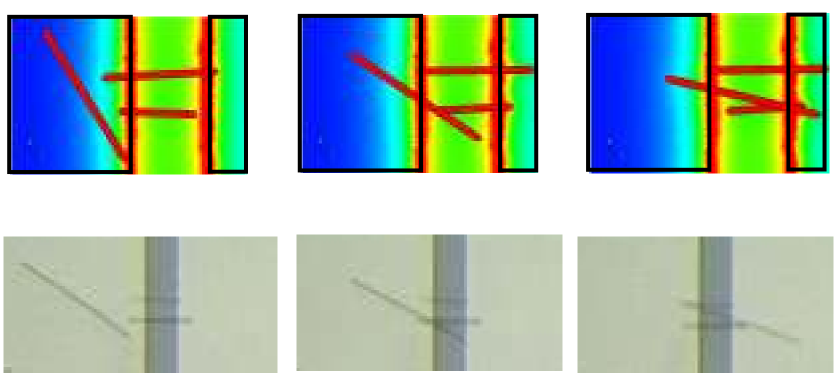
## Snap shorts of cross-linking process



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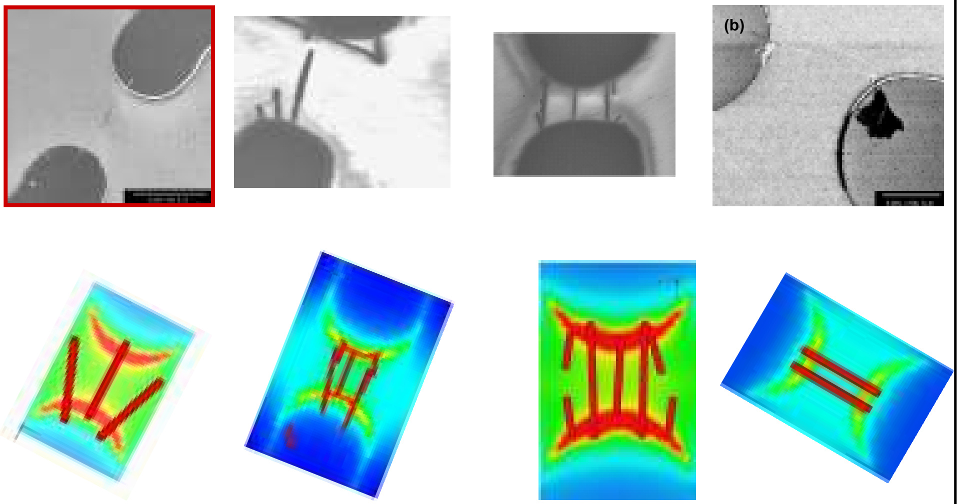
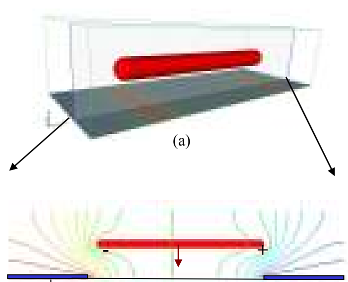
# Simulation vs. experiments

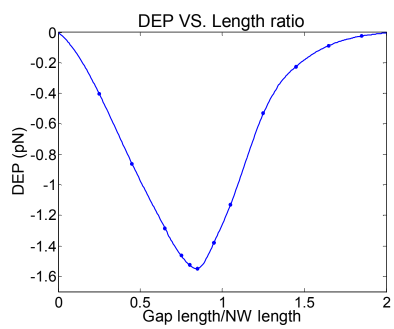



Single deposition | Failure single deposition | Symmetric multiple deposition | 2 NWs deposition



# Sorting upon nanowire lengths

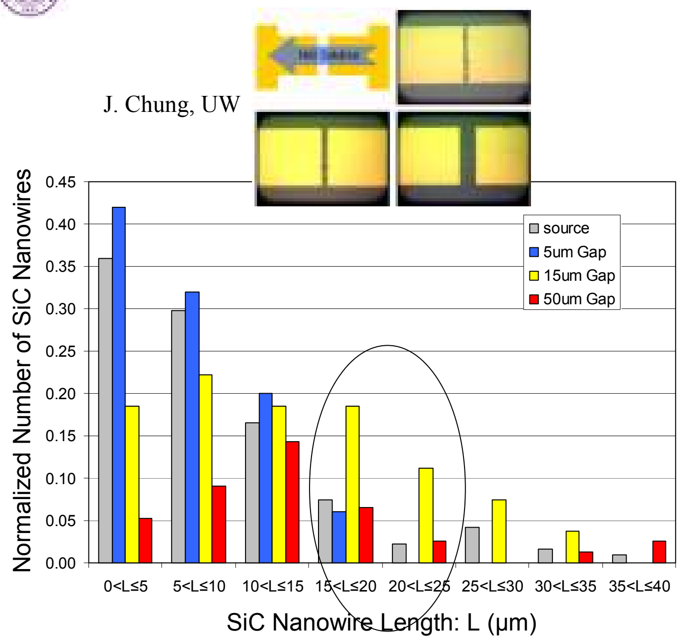



(c)

- A NW aligns across a pair of parallel rectangular-shaped electrodes;
- The DEP force on a NW varies with gap sizes. The nominal e-field strength is kept at 0.5v/μm. DEP force is maximum at a ratio ~0.8.

# Sorting upon nanowire lengths




Average NW length

NW Source: 10.4µm

5µm gap: 8.27µm

15µm gap:13.91µm

50µm gap: 17.08µm

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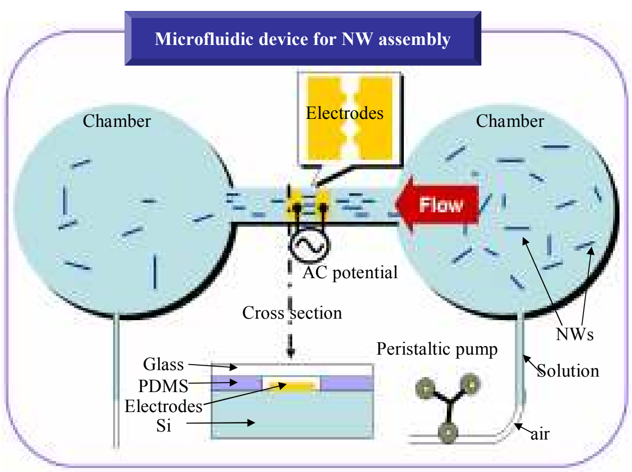
# Fluid flow assisted dielectrophoretic assembly

Both fluid flow and an AC field are controlled to achieve uniform patterning of nanowires




**Assembly process**

- NW suspension in solution
- NW Transport (~1mm) by fluid flow
- 1st alignment by shear flow
- Near field transport (0~5µm) by e-field
- 2nd alignment by electric dipole
- Deposition by electrostatic attraction
- Individual NW assembly

Proposed microfluidic device to combine fluid flow and e-field to assemble individual NWs

J. Chung, U. Washington , W.K. Liu, Northwestern

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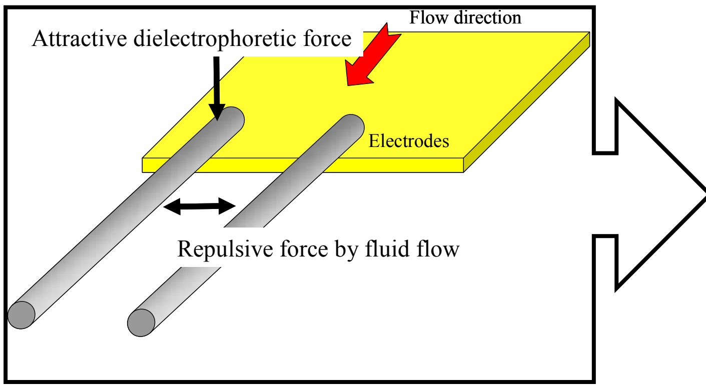
## Controlled assembly

- The dielectrophoretic force holding the SiC nanowires on electrodes was controlled to gently release, but not to lose it.
- The nanowires positioned in parallel were shifted by the repulsive fluid flow.
- As a result, the nanowires were repositioned and uniformly spaced.




**Uniform spacing is crucial for massive assembly.**

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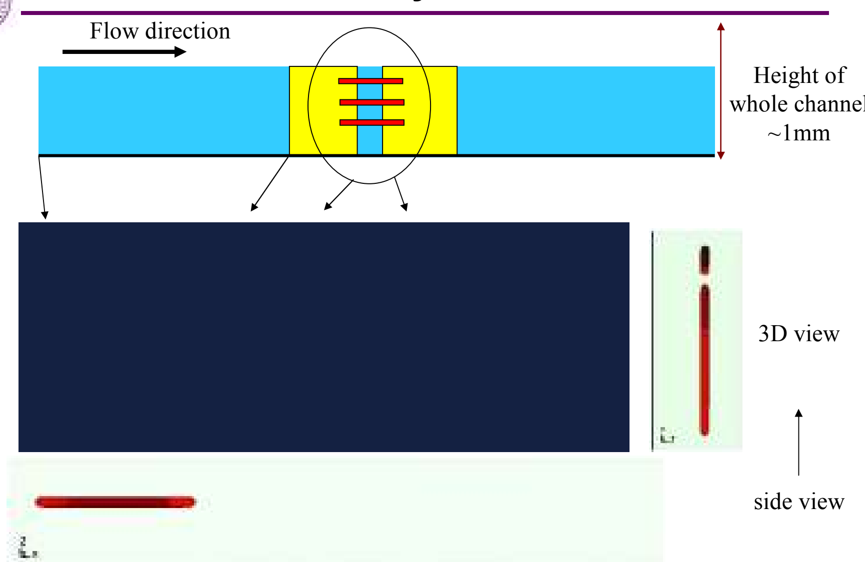
## Prediction by simulation




Pre-orientation induced by shear flow before NWs enter effective zone

Precise alignment and deposition induced by e-field at effective zone

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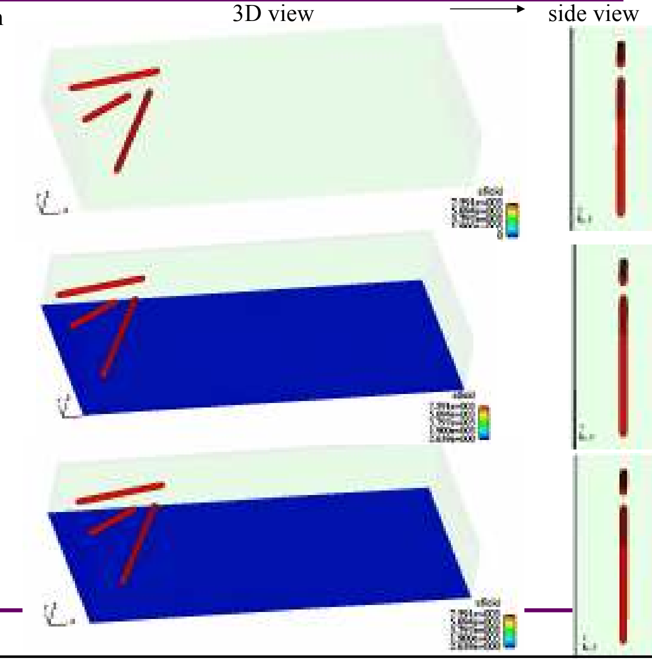
## Fluid flow dependency

Flow direction → 3D view → side view

High shear rate
$5s^{-1}$

Median shear rate
$2.5s^{-1}$

Low shear rate
$1.25s^{-1}$



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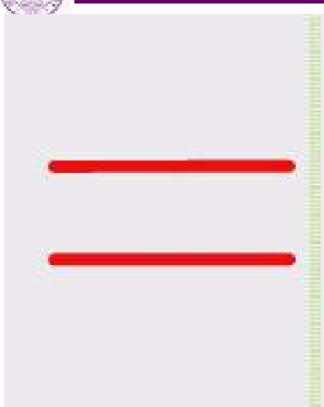
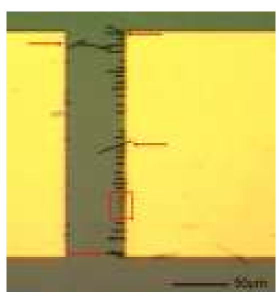
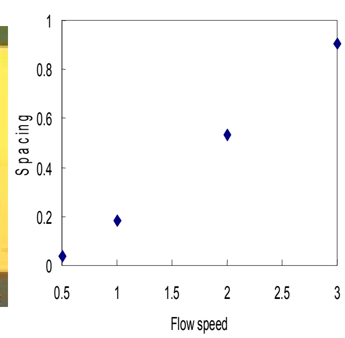
## Uniform spacing








NW spacing is normalized by 5 μ m
Flow velocity is normalized by 10 μ m/s

- ***<u>Precise control over the AC field and the fluid flow induces uniform nanowire assembly.</u>***
- ***<u>The competition between the repulsive fluid flow and the dielectrophoresis generates uniform spacing of nanowires.</u>***

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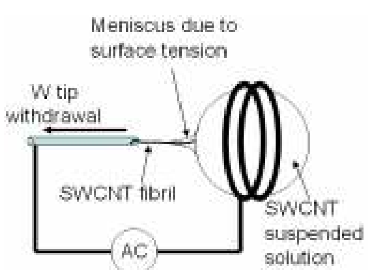
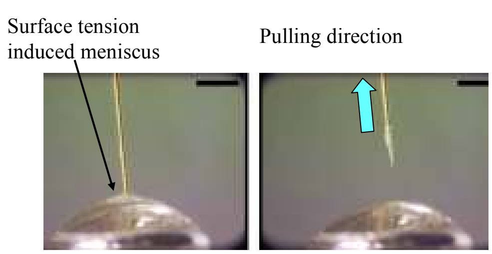
## IEFEM simulation;
## One dimensional assembly



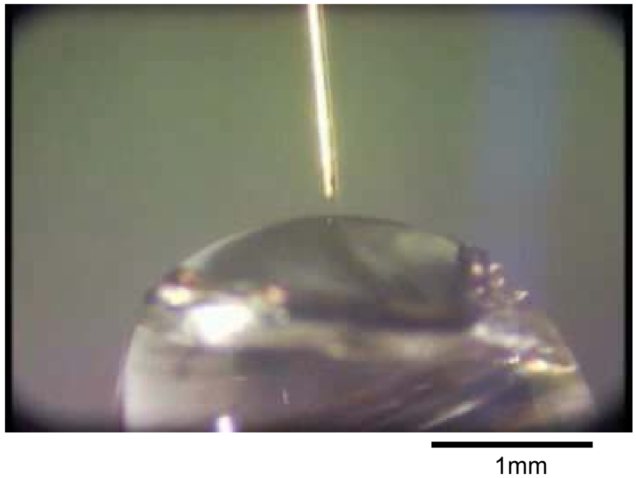
## Hybrid nanostructured materials

- Assembly using an electric field and capillary action.



# Hybrid fiber formation




The experimental process of hybrid fibril formation

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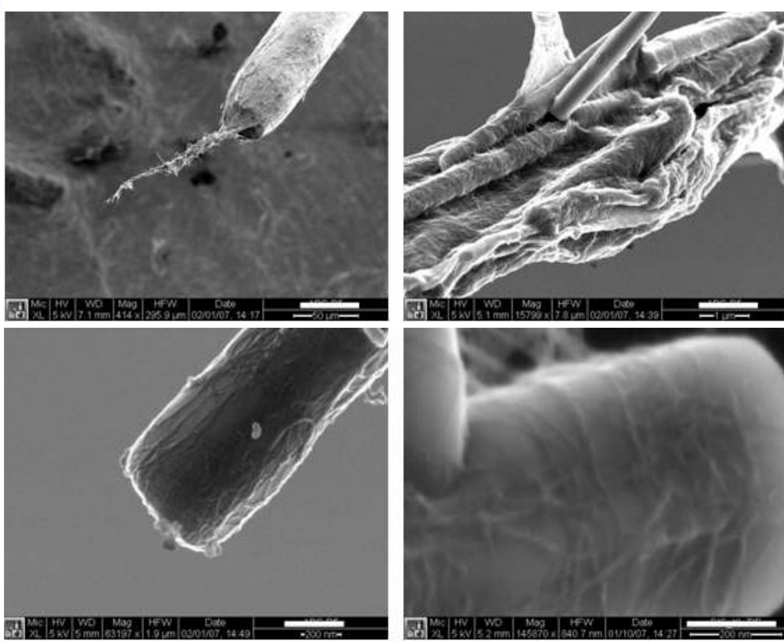
# Fabricated fiber



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## Physics involved in hybrid fibril fabrication

- Physics involved in hybrid fibril fabrication

| ***Process*** | ***Physics*** |
|---|---|
| Attraction toward W-tip | Dielectrophoresis |
| Fibril confinement and alignment | Surface tension |
| Hybrid structure formation | Van der Waals interaction |
| Continuous fibril growth | Dielectrophoresis and conductive SWCNT |

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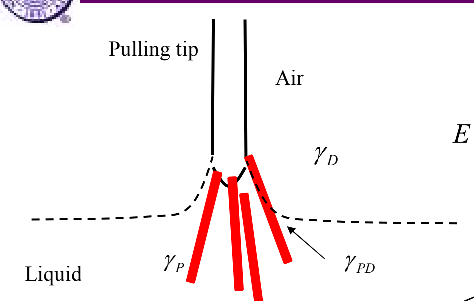
## Model the assembly process



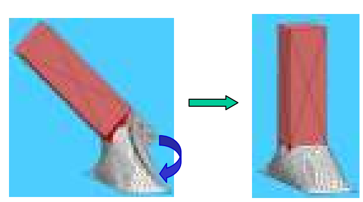

Minimization of total energy

$$E = \boxed{\gamma_D \int_D dS + \gamma_{DP} \int_{DP} dS + \gamma_P \int_P dS} + U_R + \boxed{\phi_E}$$

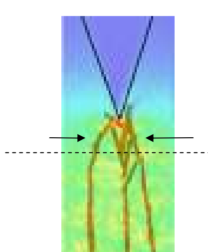
Surface tension

Electric field

Reorient NWs



Confinement



Simulation with AC field only

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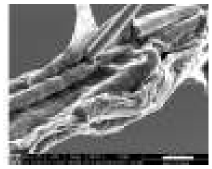
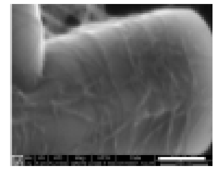
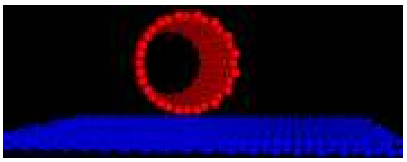
## Characterize the hybrid fibril

- The strength of hybrid fiber strongly depends SWCNT-NW bonding







Molecular Dynamics

- Tersoff-Brenner potential
  C-C: bonds, angles, torsional terms
- Lennard-Jones potential $\phi(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$
  C-SiC interaction

Modeling interaction of SWCNT-NW

$$E_{total} = E_v + \gamma l$$

Electric potential

Surface energy
=surface tension × length

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## Process parameters for controlled output

- Summary of process parameters and the controlled out-going fiber properties

| ***Process parameters*** | ***Controlled output*** |
|---|---|
| Mixing ratio | Fiber's mechanical stiffness and electrical conductance. |
| Concentration | Continuous fiber formation |
| Immersion time | Fiber's length and diameter |
| Withdrawal rate | Production speed of fibers |
| Volume of solution | Material utilization efficiency |
| Electric field | Selective attraction and orientation |

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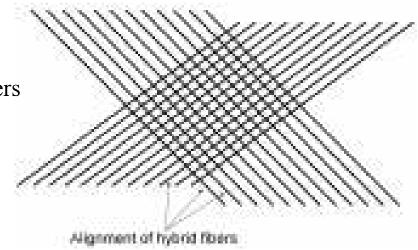
## Future work: Tunable Composite Materials

Texture of hybrid fibers




- Unique features of the composite material
  - Tunable mechanical & electrical property
  - The fiber structure is controlled by the concentration of NWs and SWCNTs
  - Good candidate for Bio-application
- Understand formation process and characterize mechanical performance?

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## IEFEM simulation; Biomaterial manipulation

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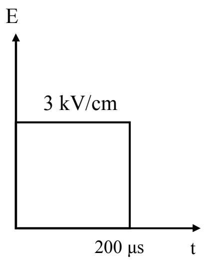
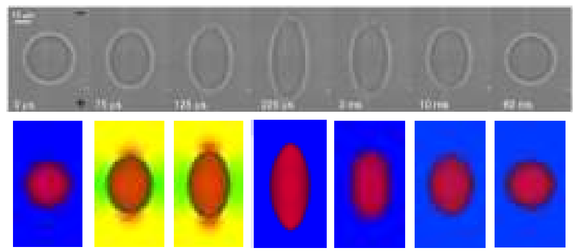
## Electrodeformation of deformable particle

Electro-Deformation and Poration of Giant Vesicles under an e-field of 3 kV/cm, with a duration of 200 μs



Riske et al., Biophy J, 2005

simulation

Inner fluid (0.2M sucrose) : $\sigma_{in} = 6$ mS m$^{-1}$

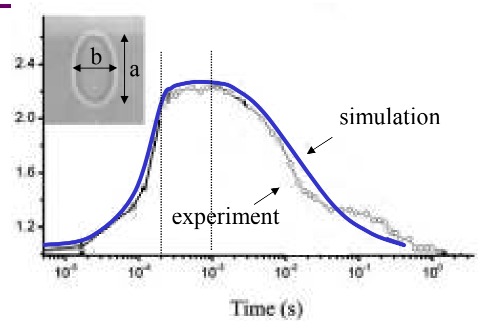
Outer fluid (0.2M glucose) : $\sigma_{out} = 4.5$ mS m$^{-1}$

Membrane modulus : 5.7 dyn/cm



## Dynamic process of electrodeformation

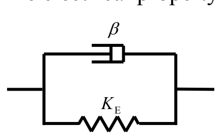
Degree of deformation (a/b) time history




•Simplified analytical model

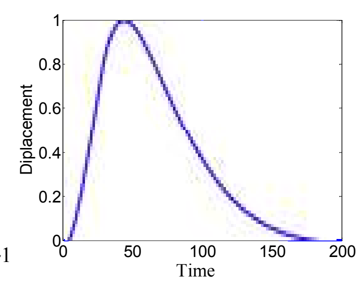
•Determine mechanical property of membrane

•Determine electrical property of cells

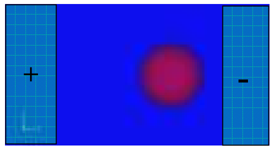


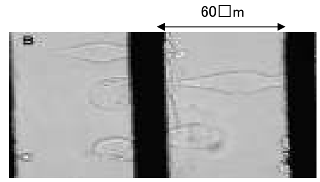

$$F(x) = K_E x + \beta \frac{dx}{dt} + m \frac{d^2 x}{d^2 t}$$

Re~1



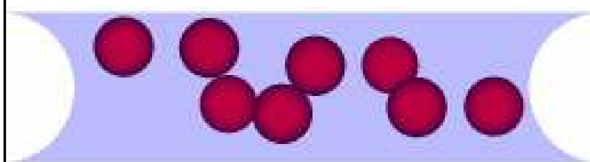
## Electrodeformation and patterning of cells

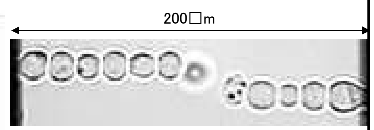



murine myeloma cells

Zimmermann et al., IEEE Plasma, 2000






2MHz AC field of 250V/cm

Hybridoma cell Diameter ~20□m

Alignment and deformation of cells induced by electric field

Zimmermann et al., IEEE Plasma, 2000

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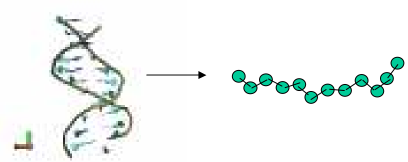
## DNA stretching

DNA in solution : coiled form

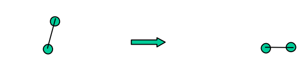
DNA in sequencing: stretched form



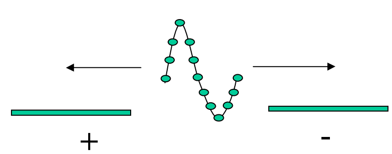
Base-pair model

Worm-like chain model of DNA immersed in liquid

- AC electrokinetic-induced conformational changes of long molecules
  - Electrokinetic force : orientation force



  - Electroosmotic flow : elongation force

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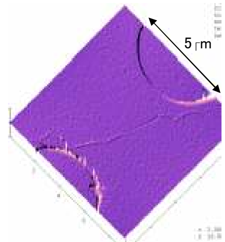
# DNA stretching (cont'd)

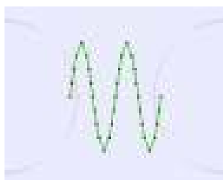

DNA motion driven by coupled fluid/electric field

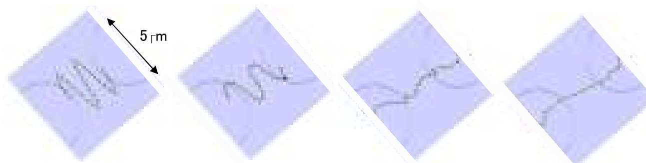
J. Chung, UW




(b)

J. Chung, UW





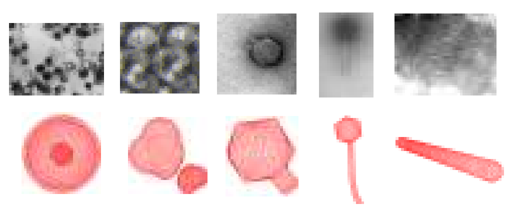

(a)

The stretching of a DNA chain between two semi-spherical shaped electrodes.



# Virus Detection

- Virus detection
  - Transportation of virus by nanofluidic channel
  - Selective deposition of virus according to sizes & electrical properties



(a) Herpes simplex virus (HSV) (b) Influenza virus (c) Bacteriophage P22 (d) Bacteriophage UrLambda (e) Inovirus

**Physical properties of the viruses**

| | Head size, nm | Tail size, nm | Total length, nm |
|---|---|---|---|
| Herpes simplex virus | | | 250 (membrane included) |
| Influenza virus | | | 100 |
| Bacteriophage P22 | 60 | 20 | 80 |
| Bacteriophage UrLambda | 50 | 150 | 200 |
| Inovirus | | | 85~280 (length)<br>10~16 (diameter) |

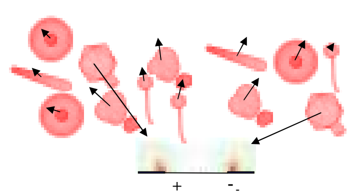
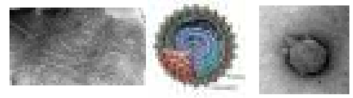


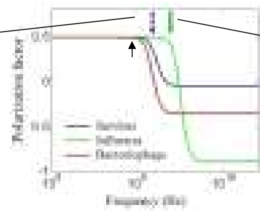

Illustration of using frequency-dependent DEP force to sort different types of viruses.

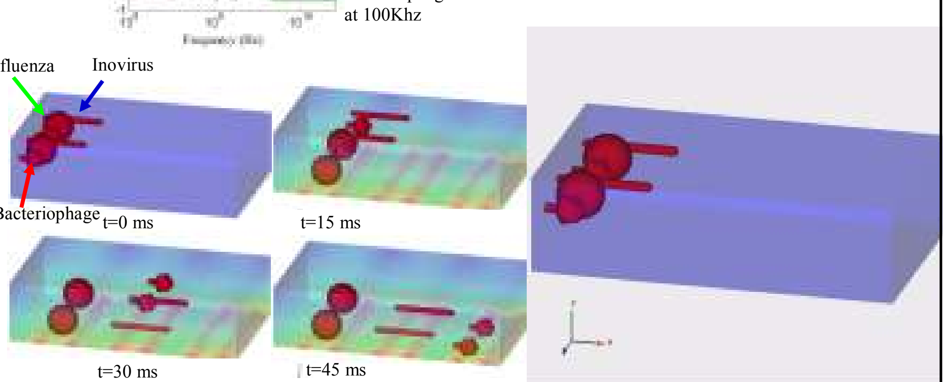
# Virus Detection (cont'd)

- Virus detection
  - Selective deposition of three different types of virus according to electrical properties



| | Inovirus | Influenza | Bacteriophage |
|---|---|---|---|
| Size (nm) | 85~280 (length) 10~16 (diameter) | 100 (diameter) | 65 (in length) |
| Permittivity | 70 | 3 | 30 |
| Conductivity (mS/m) | 8 | 80 | 3 |

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