Effects of Memory of Polarization Interactions during Particle Transport Induced by One Gradient AC Electric Field

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ABSTRACT

Molecular dynamics (MD) simulations are performed of neutrally buoyant particles in corn oil in a gradient ac electric field generated by a spatially periodical electrode array. According to the simulation, particle instability exists in the corn oil, anisotropic polarization interactions among the particles have memory, the memory is still kept even when the particles are transported by a dielectrophoresis (DEP) force, and the memory leads to formation of island-like structures in the lower electric field area, which is in good agreement with our experimental observations reported at the Nanotech 2008. We expect that full spectra of MD data for suspensions of particles from low to high concentrations would provide complete physical pictures about the particle instability, formation of island-like structure and suppression of particle instability for a variety of suspension concentrations.

Key Words: memory of anisotropic polarization interaction, gradient electric field, DEP transport, cell sorting

1 INTRODUCTION

Anisotropic interactions among polarized particles in a *uniform electric field* have been well studied and found broad applications [1-4]. Today's LCD device everywhere is one typical example [1]. Here, we will report our findings via the MD simulations that the anisotropic interactions among polarized particles have memory in a *gradient electric field* and the memory is kept even when these particles are transported by the gradient electric field.

The MD simulation is motivated by tantalizing experimental phenomena we observed and reported at the Nanotech 2008. These observations are summarized as follows. First, when neutrally buoyant poly alpha olefin particles in corn oil were exposed to a gradient ac electric field generated by a spatially periodic electrode array described in Ref. [5], the particles experienced the negative DEP and instability in all the suspensions of concentration from 0.01% to 25%. Secondly, there exists a critical initial concentration of 1%; below the critical value, the particles in the corn oil formed island-like structures; otherwise, no Island-like structure was formed. Thirdly, enough free space is a critical condition for particles to form the island-like structure. Fourthly, the island-like structures were suspended in the lowest electric field area above each grounded electrode. Finally, for the suspension of concentration of 1.126%, particles initially formed one uniform strip above each grounded electrode responding to the gradient ac electric field. When some particles were removed from one end of one grounded electrode by the electric field edge effect, the initial uniform particle strip became *wavy*.

In this report, we will describe the MD simulation method, present important simulation results, compare the simulations with our experiments, and address challenges in the MD simulations and possible solutions. Also, we will introduce one application of our findings in cell sorting.

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2 MD SIMULATIONS

2.1 Governing Equation

As shown in Figure 1, because the Brownian force and the effective gravitational force on Particle i are negligible, only the electric forces ($\boldsymbol{F}_i$) and the Stokes' drag force govern behaviors of the suspension of neutrally buoyant particles and corn oil subjected to a gradient ac electric field. So the governing equation can be written as

$$m\frac{d^2\mathbf{r}_i}{dt^2} = \mathbf{F}_i - 3\pi\eta d\frac{d\mathbf{r}_i}{dt} \tag{1}$$

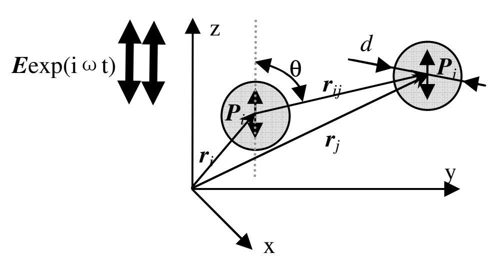

Figure 1: Two dielectric particles in an AC electric field.

In Eq. (1), m is the particle mass, d the particle diameter and η the viscosity of corn oil. $\boldsymbol{F}_i$ denotes all the electric forces on the i-th particle of

$$\boldsymbol{F}_i = \sum_{i \neq j} \boldsymbol{f}_{ij} + \boldsymbol{f}_{idep} + \boldsymbol{f}_{ie},$$

where $\boldsymbol{f}_{ij} = -\frac{\partial \Phi_{ij}}{\partial r}\boldsymbol{e}_r - \frac{1}{r}\frac{\partial \Phi_{ij}}{\partial \theta}\boldsymbol{e}_\theta$ where

$$\Phi_{ij} = \frac{1}{4\pi\varepsilon_0\varepsilon_f}\left(\frac{\boldsymbol{p}_i \cdot \boldsymbol{p}_j}{r_{ij}^{\;3}} - \frac{3(\boldsymbol{p}_i \cdot \boldsymbol{r}_{ij})\ (\boldsymbol{p}_j \cdot \boldsymbol{r}_{ij})}{r_{ij}^{\;5}}\right),$$

$\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$ and $\boldsymbol{p}_i = 4\pi\varepsilon_0\varepsilon_f\left(\frac{d}{2}\right)^3 \mathrm{Re}(\beta)\boldsymbol{E}_{rms}$.

$\boldsymbol{f}_{ij}$ is the non-zero time-average dipole-dipole interaction force on the i-th particle from the j-th particle.

$$\boldsymbol{f}_{idep} = 2\pi\varepsilon_0\varepsilon_f\left(\frac{d}{2}\right)^3 Re(\beta)\ \ \nabla E_{rms}^2(\boldsymbol{r}_i)$$

is the non-zero time-average DEP force from the gradient ac electric field, and $\langle \boldsymbol{f}_{ie}\rangle = \langle q\boldsymbol{E}(\boldsymbol{r}_i)\rangle$, the electrophoretic force on the i-th particle. In the above equations, Re (β) is the real part of the dielectric mismatch factor $\beta=(\varepsilon_p-\varepsilon_f)/(\varepsilon_p+2\varepsilon_f)$ between the particles and corn oil, ε_p and ε_f the dielectric constants of the particles and corn oil, respectively, $\boldsymbol{E}$ the ac electric field amplitude, and ε_0 the vacuum permittivity

2.2 Simulation Domain

Shown in Figures 2A and 2B are the electrode array in the chamber and the simulation domain that is naturally chosen as 7.2x3.6x3.0 mm for the MD simulation. Because the electrode length is much longer than the gap between two electrodes, it is reasonably assumed that the electric field only distributes in the Y-Z plane. The Laplace equation is solved in the simulation domain with the finite difference method and the boundary conditions for the Laplace equation were discussed in Ref. [6]. The computed electric field is plotted in Figure 2C that will be directly used for the simulation because the difference between the dielectric constants of the particles and the corn oil is small. Trajectories of particles are calculated by using a converging electric field obtained at the calculation beginning. All the parameters for the simulations are the same as those in Ref. [5]. Detailed description of the simulation method is in Ref. [7].

2.3 Simulations and Discussions

The simulations have quantitatively reproduced our experimental findings of formation of island-like structures in the lower electric field region. Shown in Figure 3 is a typical evolution sequence of particle configuration with time after a suspension was exposed to a gradient ac electric field.

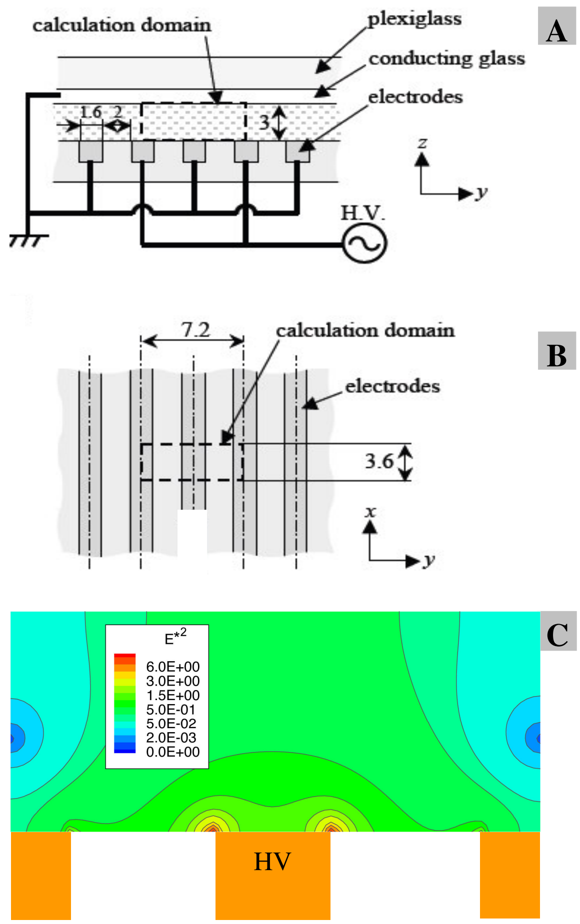

Figure 2: A: Cross section view of the electrode array in the chamber. B: Top view of the electrode array in the chamber. C: Distribution of the square of electric field strength (E^2) in the simulation domain.

The upper sequence in Figure 3 is the cross section view of the particle configuration, and shows that the particles are leaving the high field area around the HV electrode for the lower field area shown in Figure 2C; general moving direction of the particles is for the lower field area under the action of the DEP force. Interestingly, a clear particle front formed after the electric field was applied for 10 ~ 20s. At about 40 second, the particle front was broken down into two parts and each part was further becoming shorter with time and its particles were approaching to the lowest field area above each grounded electrode. The upper sequence emphasizes effects of the DEP force.

The lower sequence in Figure 3 is the top view of the particle configuration, and shows that there are a series of short chains, in parallel and perpendicular to the electrode, above each grounded electrode. Although these chains are becoming shorter with time, the distance between the two chains was kept hardly changed till all the particles were collected into the lowest field area. The lower sequence emphasizes effects of the dipole-dipole interactions among the polarized particles. The evolution sequence completely reproduces how island-like structures were being formed

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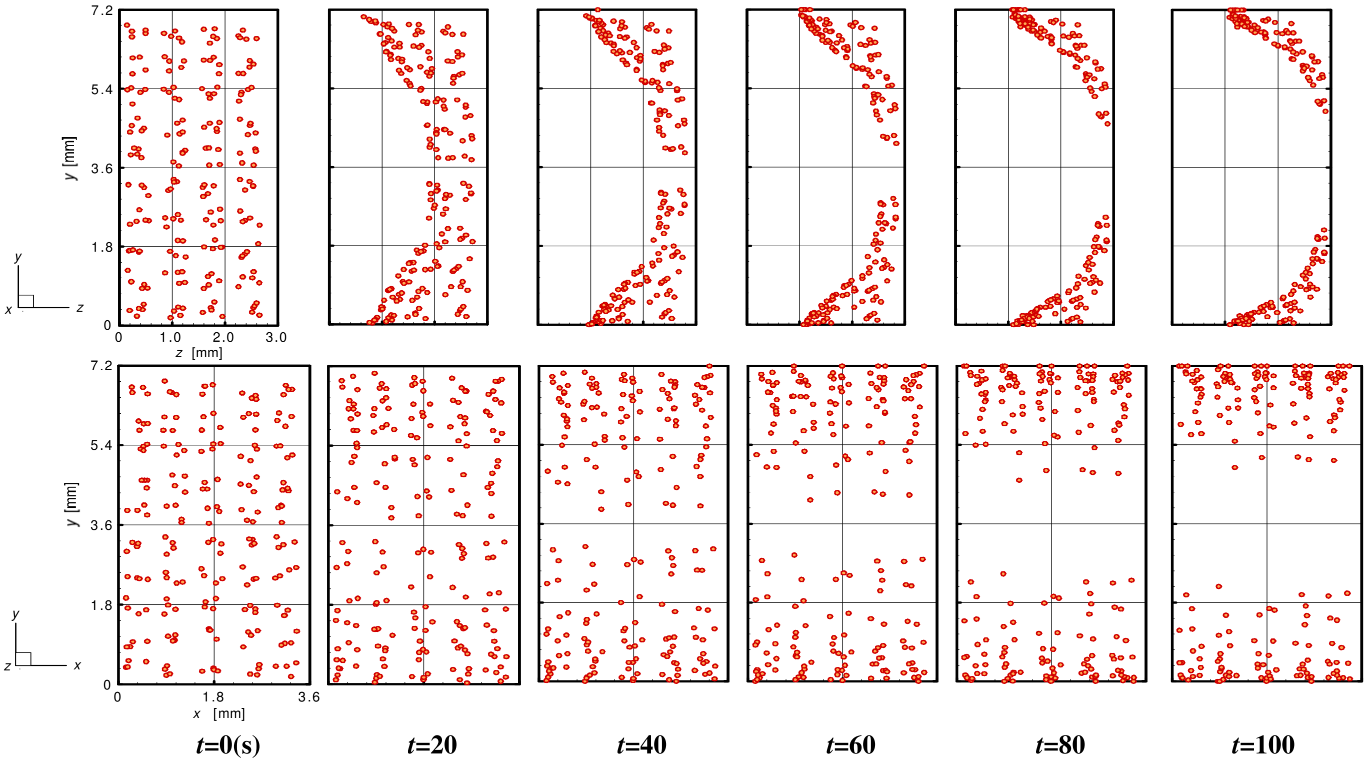

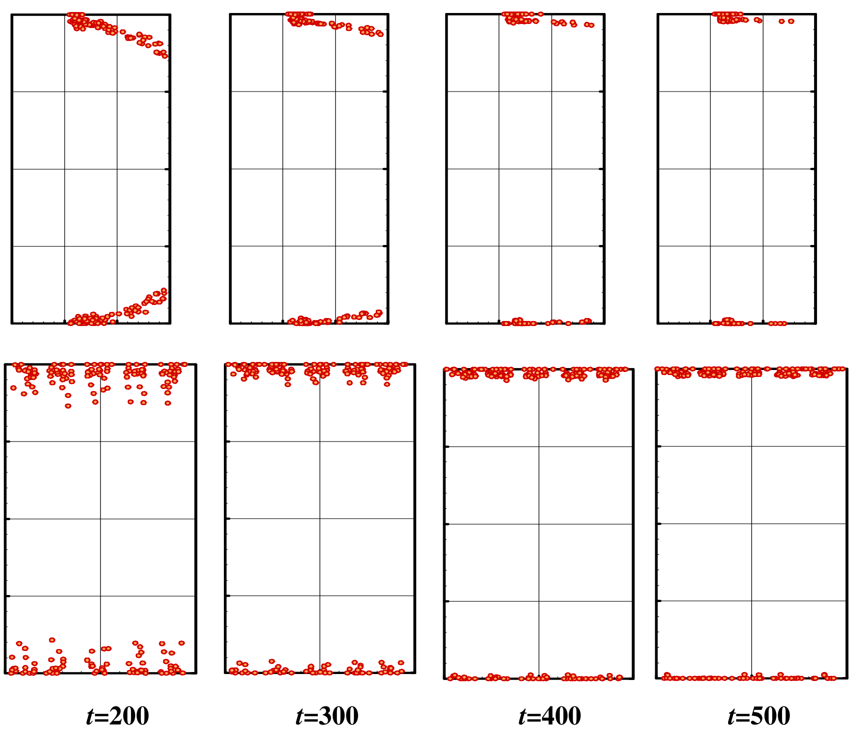

Figure 3: Evolution of particle configuration in a gradient ac electric field with time. In this simulation, the applied voltage is 5kV/100Hz, the particle volume fraction is 0.001, the relative dielectric constants of the particles and corn oil are 1.820 and 2.881, respectively, and Re (β) is -0.143. The viscosity of corn oil is 0.060 Pa s, the particle diameter is 86.7μm and the density of the particles or corn oil is 0.92g/cm^3.

we experimentally observed and reported at the Nanotech 2008 [5].

The simulations uncover that anisotropic interactions among the polarized particles have memory in a gradient electric field and that the memory is kept even when the particles are transported by the gradient electric field. The island-like structures can be regarded as signature of the memory.

To better understand the memory and its effects of dynamics, we present basic physics pictures about interactions among the polarized particles of one two-body system or one multi-body system, in a uniform external electric field or a gradient external electric field.

As shown in Figure 4, given one two-particle system in a uniform electric field, we assume that one particle, called the host particle, is located on the common tip of two 110° cones that share a symmetric axis along the electric field; when the other particle, called the guest particle, is located inside each cone, there exists an attractive interaction between them and the two particles will approach to each other and align along the electric field; otherwise, there exists a repulsive interaction between them, and the two particles will be driven away from each other. And so the two cone surfaces act as the critical interfaces

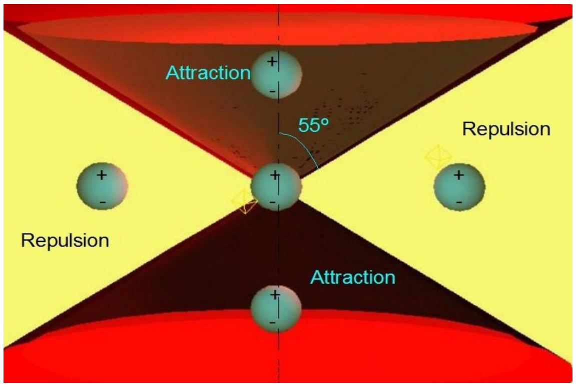

Figure 4: Critical interfaces that separate the attractive zone (Red) from the repulsive zone (Yellow) for one two-particle system in a uniform external electric field.

that separate the repulsive zone from the attractive zone for the two polarized particles [2-3]. It is the critical interfaces that are responsible for anisotropic properties of polarization interactions.

Given one multi-particle system in a uniform external field, critical interfaces may not be perfect cone surface but they do exist. There are multi-attractive and repulsive zones. So the system will not be stable. If one guest particle is in one attractive zone, it will be attracted to one host particle and align with it along the electric field; otherwise, the guest particle will be driven away from the host particle till the guest particle finds another attractive zone and aligns with another host particle along the electric field. As a consequence, many chains are formed in parallel along the electric field [2-4].

Even given one two-particle system in a non-uniform electric field, critical interfaces will not be perfect cone surfaces either because the particle dipole moment becomes location dependent; however, there still exist the critical interfaces. Given an instant, there are the critical interfaces that separate the attractive zone from the repulsive zone for the two particles. Because no particle can be stably located on the critical interfaces, the particles must experience instability. Compared with particles in a uniform electric field, particles in a non-uniform electric field will feel *one* more force, the DEP force, from the gradient electric field.

Given one multi-particle system like the suspension of neutrally buoyant particles in corn oil we studied in simulation and experimentally, when it is exposed to a gradient electric field, the particles are involved in collective motion. On the one hand, some particles form short chains due to the dipole-dipole interactions; the other hand, individual particles or short chains are transported by the DEP force; in the mean time, the DEP force some times do a favor for particle chaining, other time it takes some particles away from some short chains. No matter what the DEP force does for individual particles or short particle chains, particles are always finding their attractive zones and polarization interactions are still anisotropic there to cause particle instability. In more plain words, anisotropic interactions among the polarized particles have memory; even when individual particles or short particle chains are transported by a strong, weak or extremely weak DEP force. As the experiments [5] and the simulations have verified, it is because the anisotropic interactions among moving polarized particles have the memory, distances between the two chains in parallel are kept hardly changed till all the particles are collected around the lower field area to form isolated island-like structures.

3 CONCLUSIONS AND FURTHER WORK

In physics, we uncovered that *anisotropic interactions among polarized particles have the memory*. The memory is kept even when the particles are transported by the DEP force. The memory is responsible for formation of the isolated island-like structures. *The island-like structures can be regarded as signature of the memory*. The memory of anisotropic interactions among polarized particles has profound implications to many dynamics processes in nature, according to our reference survey.

In application, our finding is being employed to separate dead human breast cancer cells from live ones before perfusion into a single microvessel to study their adhesion *in vivo* [8]. Also, our findings will be used as online monitor of cell live state after they are electroporated. Because there is detectable difference between dielectric properties of dead cells and live cells in media, it is expected that online cell sorting would be realized.

We need developing new methods for simulations of suspensions of high concentration as the MD method requires too high computing capacity for simulating such suspensions, which will be our focus in the future work.

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REFERENCES

[1] Jos van Haaren, Nature, 392, 331, 1998.
[2] Thomas C. Halsey, Science, 258(5083), 761, 1992.
[3] Thomas C. Halsey and James E. Martin, Scientific American Magazine, Pages 58-64, October 1993.
[4] M. Whittle and W. A. Bullough, Nature 358, 373, 1992.
[5] Z.Y. Qiu, Y. Shen, S. Tada and D. Jacqmin, Nanotech, 3, 308, 2008.
[6] Z.Y. Qiu, N. Markarian, B. Khusid, and A. Acrivos, J. Appl. Phys., 92, 2829, 2002.
[7] S. Tada, Y. Shen and Z. Qiu, Nanotech, 3, 390, 2008.
[8] B. Fu and S. Shen, VEGF-induced Microvessel Hyperpermeability Increases Cancer Cell Adhesion in vivo, FASEB J., 2004.