Trapping force on a finite-sized particle in a dielectrophoretic cage

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The point dipole (PD) model is routinely used for estimating the dielectrophoretic (DEP) force acting on a particle placed in the nonuniform electric fields of dielectrophoresis devices, such as square cages. We show that if the particle size is much smaller than the dielectrophoretic cage size, the PD model accurately approximates the actual DEP force, computed numerically using the Maxwell stress tensor method. However, when the two sizes are comparable, the actual DEP force differs significantly in both magnitude and direction from that given by the PD model.

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In recent years, primarily due to improvements in the microfabrication techniques, many new applications of dielectrophoresis have been developed for the handling of micron and nanosized particles. For example, dielectrophoresis has been used for separating submicron-sized latex spheres and viruses [1,2], separating DNA molecules and proteins [3], characterizing and separating bacterial cells [4,5], removing cancer cells from human blood [6–8], and trapping submicron sized particles in cages with dimensions comparable to the particles size [9,10]. Our focus in this paper is on the contact less trapping force acting on a particle placed in a dielectrophoretic square 3D cage which in the past has been estimated using the point dipole (PD) model [11–15]. The goal of the present study is to compute the actual force in this configuration and determine the validity of the PD model.

A simple 3D dielectrophoretic cage can be formed by placing four electrodes in the four side walls of a square shaped channel, as shown in Fig. 1. The voltages of the four electrodes are selected such that the electric field magnitude is locally minimum at the center of the domain where one wishes to attract and hold the particle. This device is of practical interest as it provides a way to trap a particle in a contact less fashion, at the center of the cage. The magnitude of the electric field $\mathbf{E}$ in the xz plane for the case without the particle is shown in Fig. 2(a). Notice that the magnitude is locally minimum at the cage center and increases with increasing distance from the domain center.

Figure 2(b) shows that the electric field inside the cage is nonuniform, and its gradient near the domain center is nonzero, except at the center itself where it is zero. The lines of the gradient of the electric field magnitude shown in Fig. 2(b) emanate approximately radially from the cage center and end at the edges of the electrodes. If a particle is placed in this domain and its dielectric constant is smaller than that of the liquid, it will experience the so-called dielectrophoretic (DEP) force towards the center of the domain, i.e., in the direction opposite to the lines of the gradient of the electric field magnitude. If the dielectric constant of the particle is greater than that of the liquid, the DEP force is in the direction away from the center. This situation will not be considered here, since it has limited practical applications as in this case the particle will not be trapped at the center of the cage in a contact less manner.

An estimate of the trapping force can be obtained using the PD model which considers the particle as a point dipole and thus assumes that the gradient of the electric field is approximately constant over the particle. According to the PD model, the dielectrophoretic force acting on a linearly and homogeneously polarizable spherical particle placed in a dc electric field is given by the expression $\mathbf{F}_{DEP,PD}=4\pi a^3\varepsilon_0\varepsilon_c\beta\mathbf{E}\cdot\nabla\mathbf{E}$, where a is the particle radius, $\varepsilon_0=8.8542\times10^{-12}$ F/m is the permittivity of free space, $\mathbf{E}$ is the electric field, and $\beta=(\varepsilon_p-\varepsilon_c)/(\varepsilon_p+2\varepsilon_c)$ is the Clausius-Mossotti factor, ε_c and ε_p are the dielectric constants of the liquid and particle. We will assume that the particles and liquid are both perfect dielectrics. Our results are also applicable to ac electric fields, provided the rms value of the electric field is used, β is replaced by the real part of the complex frequency dependent Clausius-Mossotti factor and the force is the time averaged force. We will also present some results where the DEP force is estimated using the quadrupole model [11,15].

Clearly, when the size of the particle being trapped is comparable to the cage size, the PD model is expected to be in error because the assumption made on the electric field nonuniformity (i.e., the nonuniformity is modest and its scale is large compared to the particle size) is no longer valid and also because the presence of the particle modifies the overall electric field distribution in the cage, as the distance between the particle and the cage walls is comparable to the particle size [10]. To correct this error, the electric field must be obtained by including the particle in the electric field problem, as was done in [10] for the two canonical cases of a cylindrical particle in a cylindrical shell and a spherical particle in a spherical shell. It has been noted in the past that the error in the DEP force due to the assumptions made on the electric field nonuniformity can be reduced by incorporating the quadrupole, and if needed, additional higher order terms [11,15]. However, the error due to the modification of the electric field *cannot* be fully corrected by simply adding the higher order multipolar terms, as these terms are evaluated using the electric field computed without the particle. We make this point by presenting some results where the quadrupole terms are also included for estimating the DEP force. It is worth noting that in the uniform electric field case, the method of image can be used to determine the modified elec-

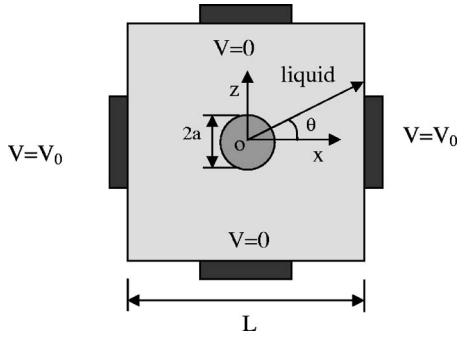

FIG. 1. A schematic of the dielectrophoretic cage used in our simulations. The cage size is L and the radius of spherical particle is a. The cage depth in the y direction is also L. The voltage applied to the electrodes in the side walls (shown in black) is denoted by V.

tric field when a particle is placed close to an electrode or a wall, but the electric potential boundary conditions in the cage are quite complex which makes the use of the method of image difficult. In this paper, the actual DEP force is computed numerically by solving Laplace's equation for the dielectric continuous medium, with appropriate boundary conditions, and then integrating the Maxwell stress tensor (MST) over the particle's surface. This actual value of the DEP force is compared with the value given by the PD and quadrupole models.

COMPUTATIONAL APPROACH

Let us denote the domain containing a liquid and a solid particle by Ω, the interior of the particle and its surface by $P(t)$ and $\partial P(t)$, respectively, and the domain boundary by Γ. To calculate the electric field $\mathbf{E}$, we first solve the electric potential ϕ problem in Ω: $\nabla\cdot(\varepsilon\nabla\phi)=0$ with the boundary conditions on the particle surface given by $\phi_1=\phi_2, \varepsilon_c(\partial\phi_1/\partial n)=\varepsilon_p(\partial\phi_2/\partial n)$ on $\partial P(t)$ where ϕ_1 and ϕ_2 are the electric potential in the liquid and particle. The electric potential is prescribed on the electrodes as constant values and the normal derivative of the potential is taken to be zero on the remaining domain boundary. The electric field is then deduced from the equation $\mathbf{E}=-\nabla\phi$. The Maxwell stress tensor $\boldsymbol{\sigma}_M$ is given by $\boldsymbol{\sigma}_M=\varepsilon\mathbf{E}\mathbf{E}-\frac{1}{2}\varepsilon(\mathbf{E}\cdot\mathbf{E})\mathbf{I}$, where $\mathbf{I}$ is the identity tensor and the dielectrophoretic force acting on the particle is then obtained by integrating $\boldsymbol{\sigma}_M$ over the particle surface, i.e. $\mathbf{F}_{DEP}=\int_{\Gamma_p}\boldsymbol{\sigma}_M\cdot\mathbf{n}\,d\mathbf{s}$, where $\mathbf{n}$ is the unit outer normal on the surface of the particle. In our finite element code, the domain is discretized using a tetrahedral mesh and the boundary conditions are imposed on the surface of the particle. The resulting linear system of equations is solved using a multigrid preconditioned conjugate gradient method [16,17].

The simulation results will be nondimensionalized by assuming that the characteristic length and electric field scales are L and V_0/L, respectively, where V_0 is the voltage of the energized electrodes (see Fig. 1). The results are presented for $L=1$. The nondimensionalized electric field $\mathbf{E}'=\mathbf{E}L/V_0$ and the nondimensionalized DEP force $\mathbf{F}'_{DEP}$ is given by $\mathbf{F}'_{DEP}=L^3\mathbf{F}_{DEP}/4\pi a^3\varepsilon_0\varepsilon_c V_0^2$.

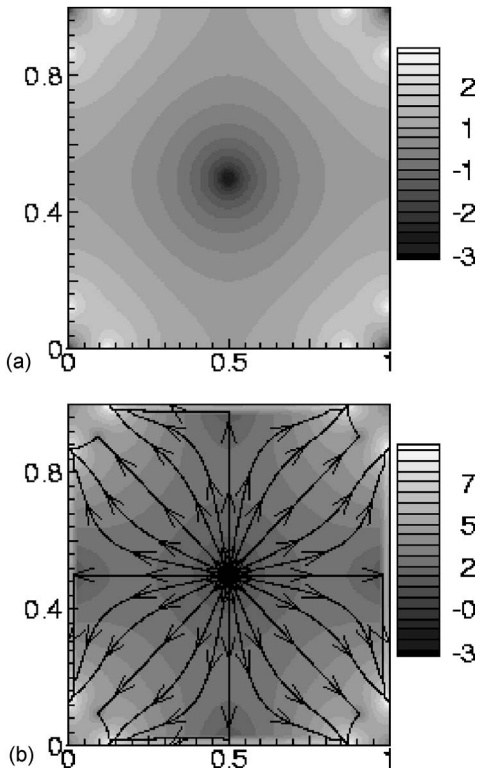

FIG. 2. E for the case without any particle placed inside the cage of Fig. 1. The electrodes are placed at the center of the side walls, and their width is $0.75L$. $V=1$ and $L=1$. The electric field does not vary with y. (a) Isovalues of $\log(|\mathbf{E}|)$. (b) Isovalues of $\log(|\nabla\mathbf{E}^2|)$ and the lines of the gradient of the electric field magnitude. A small particle with $\varepsilon_p/\varepsilon_c<1$ experiences the DEP force in the opposite direction of the arrows.

The ratio of the actual DEP force and that given by the PD model is then used to quantify the error in the point dipole model $\chi=|\mathbf{F}_{DEP}|/|\mathbf{F}_{DEP,PD}|$. The factor χ is computed for various particle radii as the cage size is held fixed. We also study the dependence of χ on the dielectric constant ratio $\varepsilon_p/\varepsilon_c$.

RESULTS

We present results for the three-dimensional cage containing a spherical particle shown in Fig. 1. The electric field magnitudes for particles of radii 0.025, 0.05, and 0.25 inside the cage are shown in Figs. 3(a)–3(c). It is clear that although the particles of radii 0.025 and 0.05 modify the electric field near them, the overall nature of the electric field in the domain remains approximately unchanged. For the larger sized particle, on the other hand, the modification of the electric field is substantial both near and away from the particle surface [see Fig. 3(c)]. Consequently, in this case, the actual DEP force cannot be determined accurately from the electric field computed without the particle, as is done in the dipole model, and therefore we expect a larger discrepancy between the actual DEP force and its estimate given by the PD and quadrupole models.

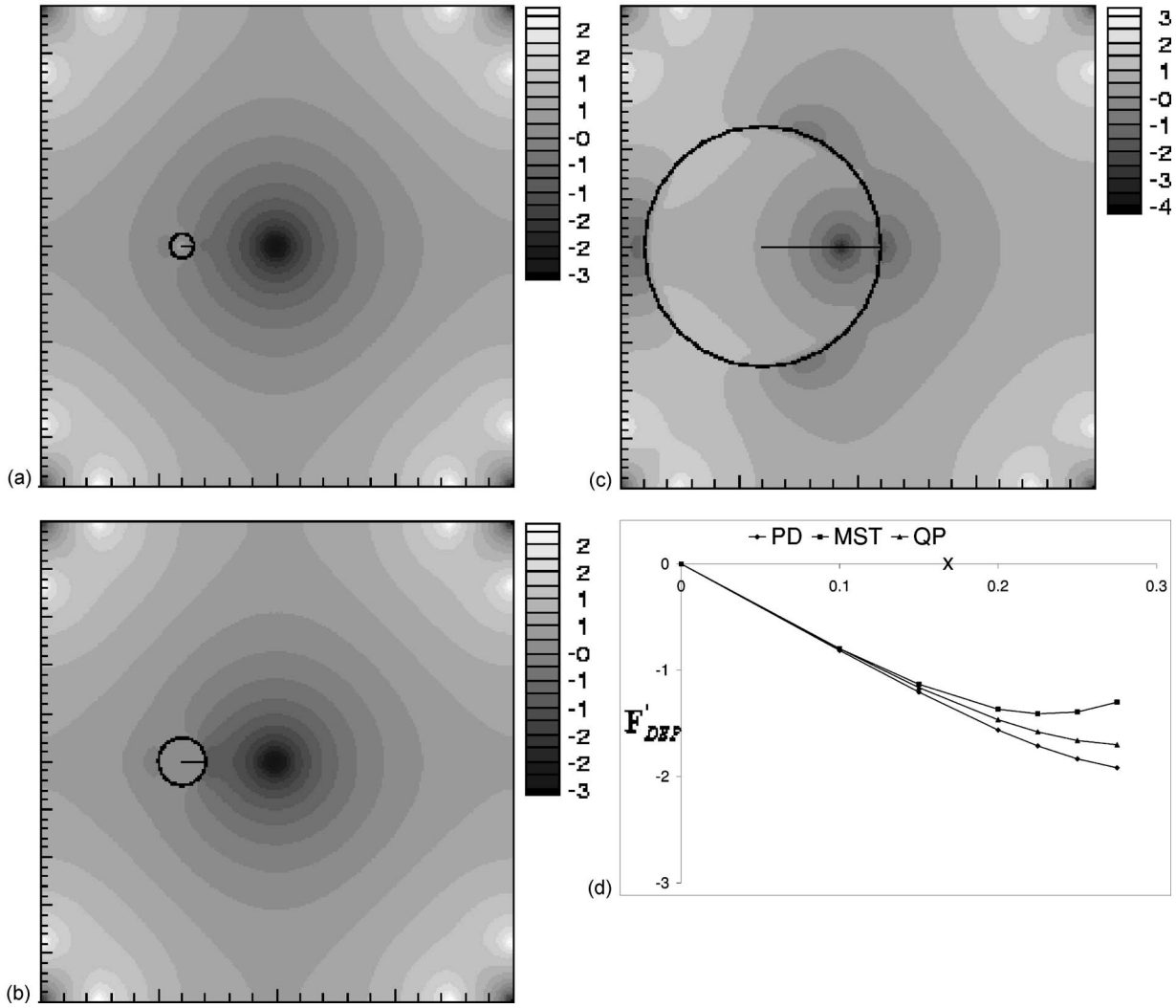

FIG. 3. Isovalues of $\log(|\mathbf{E}'|)$ in the xz plane passing though the particle center for $\varepsilon_p/\varepsilon_c=0.1$. It is clear that the electric field is modified near the particle. The particle center is at $(-0.2,0,0)$. (a) $a=0.025$. (b) $a=0.05$. (c) $a=0.25$. (d) Along the x axis, the x component of the dimensionless DEP forces for the PD and quadrupole (QP) models and the actual DEP force obtained numerically for $a=0.2$ and $\varepsilon_p/\varepsilon_c=0.1$. Notice, in particular, the fact that the DEP force decreases with x when $x>0.225$ is not correctly predicted by the PD and quadrupole models.

In Fig. 3(d), the x components of the dimensionless DEP force for the PD and quadrupole models, and the actual DEP force obtained numerically, are plotted as functions of x. For all three cases, the force is zero at the cage center ($x=0$) and negative for $x>0$. The latter implies that if the particle is moved away from the cage center, the force acts to bring it back to the center, and thus the center is a point of stable equilibrium. Also, notice that at $x=0.25$ the actual DEP force is $\sim 30\%$ smaller than the value given by the PD model, and that the quadrupole model is slightly closer to the actual value. It is interesting to note that for positive dielectrophoresis, the PD model underestimates the DEP force [10] while it mostly overestimates that force in the case of negative dielectrophoresis considered here. Furthermore, the PD and quadrupole models incorrectly predict that for $x>0.22$ the DEP force continues to increase with x.

To quantify differences between the actual DEP force and its PD approximation throughout the domain, we plot χ along three rays with $\theta=0°$, 22.5°, and 45.0° emanating from the cage center, as shown in Fig. 1. It is sufficient to only consider the distribution of DEP force in this 45° sector, as the DEP force distribution in the remaining sectors of the cage is a transformed image of the DEP force in this sector. The ray with $\theta=0°$ is along the x axis and $\theta=45°$ is along the diagonal of the cage. The actual DEP force, as well as the PD approximation, along these two directions is directed towards the center of the cage because of the symmetry of the electric field, and therefore along these two directions we only need to specify the magnitude of the DEP force (see Fig. 4).

In Fig. 4, the distributions of the actual DEP force and its PD approximation in the xy plane are shown for $a=0.2$ and $\varepsilon_p/\varepsilon_c=0.1$. Near the center of the cage the PD approximation is approximately equal to the actual DEP force. Along the x and y axes and the cage diagonals their directions are the same because of the symmetry, but their magnitudes differ.

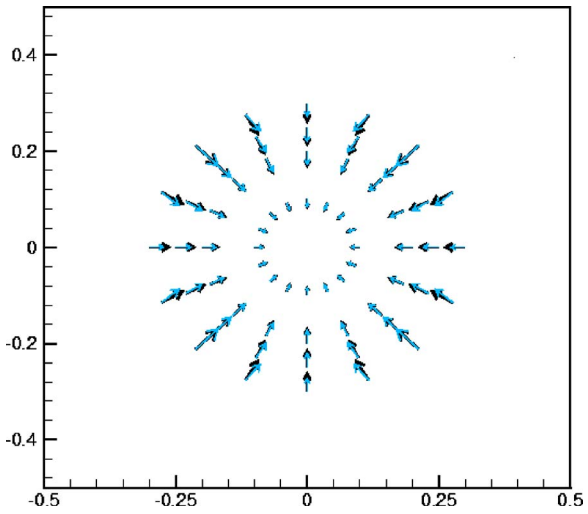

FIG. 4. (Color online) The actual DEP force (gray arrows) and its PD model (black arrows) in the xy plane for $a=0.2$ and $\varepsilon_p/\varepsilon_c=0.1$. The vectors are scaled by a constant factor. The particle center is in the domain midplane. Notice that along the x and y axes and the cage diagonals only the magnitude of the actual force differs from the PD approximation. However, along all other directions from the cage center both magnitudes and directions of arrows differ.

For any other point inside the cage, the direction, as well as the magnitude, of the actual DEP force differ from that of the PD model.

In Fig. 5(a), the ratio of the actual DEP force and its PD estimate χ is plotted along the x axis for several different

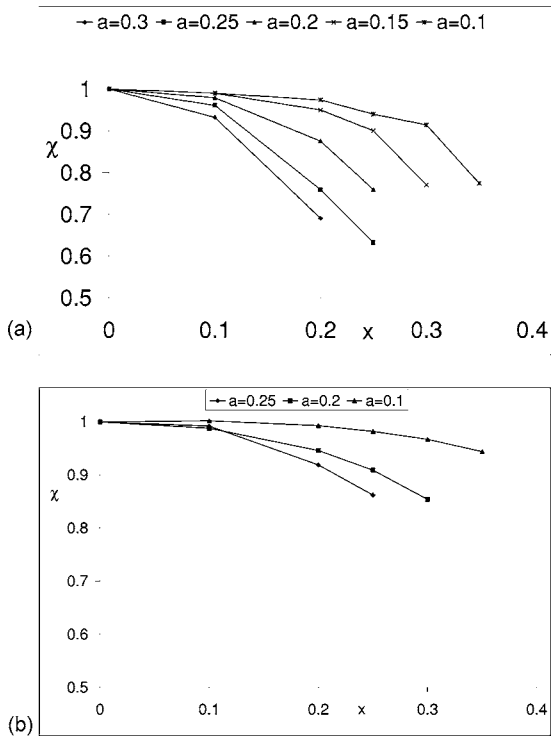

FIG. 5. χ is shown along the x axis for different values of a. Since $\chi<1$, the PD model overestimates the dielectrophoretic (DEP) force. (a) $\varepsilon_p/\varepsilon_c=0.9$ and (b) $\varepsilon_p/\varepsilon_c=0.1$.

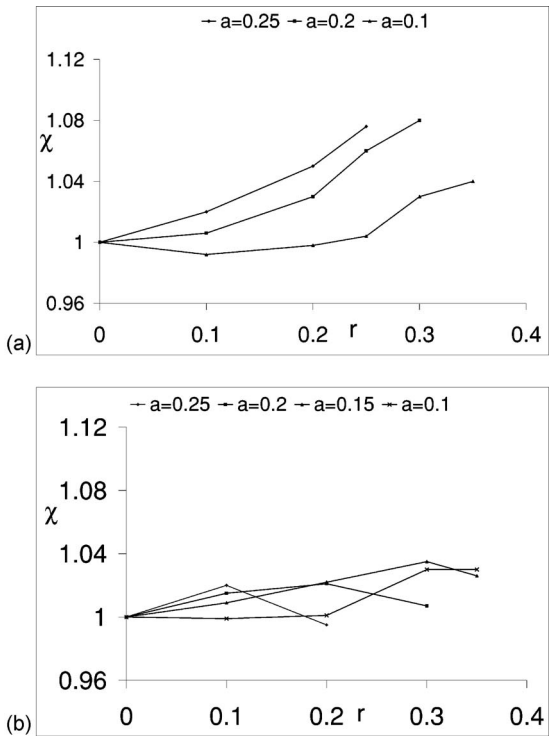

FIG. 6. χ is shown along the cage diagonal for different values of a. For most cases, since $\chi>1$, the PD model underestimates the DEP force. The increase in χ is larger for larger a values. (a) $\varepsilon_p/\varepsilon_c=0.5$ and (b) $\varepsilon_p/\varepsilon_c=0.1$.

particle radii and $\varepsilon_p/\varepsilon_c=0.9$. It is clear that as the particle radius decreases to zero, χ tends to 1, and therefore in this case the PD model provides a good estimate of the force. However, as the particle size increases, χ decreases, showing that the PD approximation clearly deviates from the actual force. Notice that for all particle radii near the cage center χ is approximately one and that it decreases with increasing x. The PD model therefore overestimates the DEP force. For example, for $a=0.25$, at $x=0.22$ the value of χ is ~ 0.86, which means that the actual DEP force is approximately 14% smaller than the value given by the PD model.

In Fig. 5(b), χ is plotted along the x axis for $\varepsilon_p/\varepsilon_c=0.1$, and several values of the sphere radius. Again, near the center of the domain χ is approximately one and it decreases with increasing x. The decrease in χ is larger than in Fig. 5(a) for $\varepsilon_p/\varepsilon_c=0.9$, and thus the error made by using the PD model is greater when $\varepsilon_p/\varepsilon_c$ is smaller. For example, for $a=0.25$ and $\varepsilon_p/\varepsilon_c=0.1$, at $x=0.2$, $\chi=0.6$ which implies that the PD model differs from the actual value by 40%. This is an important result which should be taken into account for estimating the trapping force, the time it takes to trap the particle, as well as the magnitude of the DEP force versus other forces (e.g., Brownian forces on nanosized particles).

In Fig. 6(a), χ is plotted along the cage diagonal for different particle radii and $\varepsilon_p/\varepsilon_c=0.5$. Near the center of the cage χ is approximately one, it increases with increasing distance r from the cage center, indicating that the PD model underestimates the DEP force. The increase in the DEP force, however, is small compared to the decrease along the x axis. Also notice that the increase in χ is larger for the larger sized

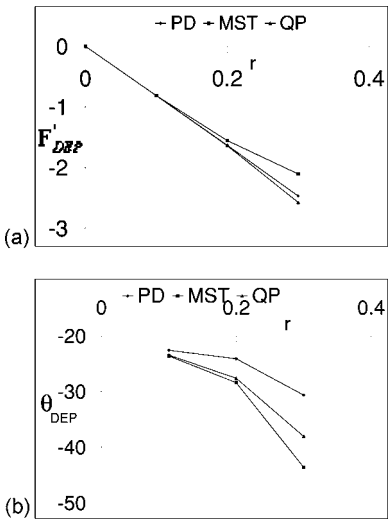

FIG. 7. The magnitude of the dimensionless DEP force and its direction θ_{DEP} are shown along $\theta=22.5°$ for $a=0.2$ and $\varepsilon_p/\varepsilon_c=0.1$. (a) The actual dimensionless DEP force, and its estimates given by the PD and quadrupole (QP) models. The PD model is closer to the exact value. (b) The directions of the actual DEP force and that for the PD and quadrupole models. The direction given by the quadrupole model is closer to the actual direction.

particles. For $a=0.2$, at $r=0.2$ the value of χ is ~ 1.03.

In Fig. 6(b), χ is plotted along the cage diagonal for a larger dielectric constant ratio $\varepsilon_p/\varepsilon_c=0.1$ and several values of the sphere radius. As above, χ increases with increasing r near the cage center, but the increase is smaller than for $\varepsilon_p/\varepsilon_c=0.5$. Also, notice that χ decreases with r, when r is larger than a critical value which depends of the particle radius.

We next discuss the direction in which the DEP force acts for a line emanating at $\theta=22.5°$ from the cage center. The force direction is investigated in terms of the angle θ_{DEP} between the DEP force and the x direction. Clearly, if $\theta_{DEP}=-22.5°$, the DEP force acts towards the center of the cage. In Fig. 7, θ_{DEP} for the actual DEP force, its PD and quadrupole approximations, and the dimensionless force magnitudes are shown for $a=0.2$ and $\varepsilon_p/\varepsilon_c=0.1$. The figure shows that away from the cage center, the magnitude and direction of the actual DEP force differ from those for the PD and quadrupole models. Notice that the magnitude given by the PD model is closer to the actual value, but the direction is closer for the quadrupole model. Also, since the magnitude of $(\theta_{DEP}+22.5°)$ is not zero for the actual DEP force, it is directed less directly towards the cage center.

CONCLUSIONS

A numerical scheme based on the Maxwell stress tensor method was used for computing the DEP trapping force acting on a spherical particle in a dielectrophoretic square cage. Our simulations show that the PD model gives an accurate estimate when the particle size is small compared to the cage size. However, for larger sized particles, the actual (computed) trapping force along the direction joining the cage center and the center of electrodes is smaller than the value given by the PD model, but it is slightly larger along the cage diagonals. Along any other ray emanating from the cage center, both magnitude and direction of the actual trapping force differ from the PD estimates. These results do not change significantly when the quadrupole term is included while estimating the DEP force, as the multipole method does not account for the fact that the presence of the particle of finite size modifies the overall electric field distribution in the cage. The discrepancy between the actual trapping force and that given by the PD model increases with the radius of the particle and decreases with the dielectric ratio $\varepsilon_p/\varepsilon_c$. For instance, the PD estimate overestimates by as much as 40% the actual value for a ratio $\varepsilon_p/\varepsilon_c$ of 10% and a particle radius which is one fourth of the side of the cage. This discrepancy should be taken into account in designing dielectrophoretic devices, which require an estimate of the trapping time and efficiency.

ACKNOWLEDGMENTS

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