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RESEARCH ARTICLE

BIONANOPARTÍCLES OF TOBACCO MOSAIC VIRUS (TMV) FORCED INTO ELECTROROTATION

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ABSTRACT

Construction and characterization of artificial microstuctures, their mechanical and electrical properties, and the response to diverse stimuli have motivated strong research interests. Nanometric objects share characteristics, which are typical for macroscopic objects at the one hand, and for 'molecular' (quantum) objects at the other. Nano machines carry out mechanical movements similar to their macroscopic counterparts, i. e. translation as well as rotation, although their driving forces are of different nature. While gravitational forces are typical only for macroscopic robots, on the nanoscale Stokes resistance and Brownian movement gain importance. The imposition of forces may occur by an external electric field, which interacts with the nano entities. The consideration of their size and real shape of the particle instead of the common ellipsoidal approach in electric field calculations should provide much more accurate results. A theoretical model is developed in this paper to provide a description of electrorotation depending on the size of a cylinder-shaped particle. It is applied in a study of the controlled rotational movement of a short cylindrically formed bioparticle, represented by the natural shape of the Tobacco Mosaic Virus (TMV) immersed in a suspending dielectric medium.

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INTRODUCTION

The manipulation of nanoparticles is a current topic of research in the nanotechnology field. To quote only few, atomic force microscopy (AFM) is widely used, where most important issues are the high-precision moving of a nanoparticle and the robustness of the control algorithm (Korayem *et al.,* 2014; Maharaj *et al.,* 2014), laser technique is applied (Tetsuhiro *et al.,* 2012; Guanghao *et al.,* 2015), and electron beam manipulation is reported where nanoparticles are trapped with the beam and move dynamically toward the location with higher electron density (Haimei *et al.,* 2012). Electric fields can induce various types of motion in liquid suspensions of colloidal nanoparticles (Cheng *et al.,* 2014; Eunpyo *et al.,* 2014).

One of the prime objectives points toward the controlled manipulation of individual atoms and molecules by displacing and combining the nanoparticles. Almost any structure with micro- or nanodimension might be assembled. Present research activities imply basic objectives, as e.g. the construction and characterization of artificial microstuctures, their mechanical and electrical properties, the chemical stability and the response to diverse stimuli. At this length scale, nanometric objects share characteristics, which are typical for macroscopic objects at the one hand, and for 'molecular' (quantum) objects at the other. In this hybride arrangement enter new phenomena to be considered: thermal noise, surface effects, quantum fluctuations, disorder and non-linearity. Most of these effects are small at a macroscopic length scale and are then treated as perturbations. At the mesoscopic length scale, these perturbations reach the importance of the main effect and their actions might be decisive. Electro rotation may be useful as a practical means of inducing rotation in molecular structures.

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Electrorotational force: Electrokinetic effects are caused by the interaction of induced dipoles with electric fields. Dielectrophoretic manipulation of particles is commonly performed on planar quadrupole electrode arrays. Observed phenomena depend on the physical properties of the electric field, the nature of particles, i.e. size, shape, and composition, as well as the electrical properties of the suspending liquid, in particular its polarizability (Midlet *et al.,* 2017; Jones, 2005; Honegger *et al.,* 2013). A variety of movements is produced by changing the nature of the alternating electric field, including attraction, repulsion and rotation.

For a given external electric field $\vec{E}_0(\vec{r})$, the polarization within a dielectric body is given by

$$\vec{P}(\hat{r}) = \varepsilon_0(\varepsilon - 1)\vec{E}_i(\hat{r}) = \varepsilon_0(\varepsilon - 1)\alpha(\hat{r})\vec{E}_0(\hat{r}), \tag{1}$$

where $\alpha(\hat{r})$ is a tensor, ε_0 is the vacuum permittivity, ε the permittivity of the particle, $\vec{E}_i$ the internal electric field, and $\hat{r}$ the position vector pointing in the direction of the electric field. The depolarization factor $\alpha(\hat{r})$ relates the internal electric field to the external field. In the case of ellipsoidal dielectric bodies, this factor is easily obtained. For a sphere e.g. it is given by $\alpha = 3/(\varepsilon+2)$. For non spherical but ellipsoidal cells, both for prolate and oblate shape, one gets for an oblate ellipsoid of radius R and length $L(R>L)$

$$\alpha = \{1 - (\varepsilon - 1)\cdot f(q)\}^{-1}, \tag{2}$$

with

$$f(q) = \left[(q^2 + 1)\left(q \cdot \arctan\frac{1}{q} - 1\right) \right], \tag{3}$$

For a prolate ellipsoid of radius R and $L>R$, the function $f(q)$ results in

$$f(q) = q^2 \left[1 + \frac{\sqrt{q^2+1}}{2} ln \frac{\sqrt{q^2+1}-1}{\sqrt{q^2+1}+1} \right] \tag{4}$$

In both cases is $q^2 = R^2/|L^2-R^2|$.

Polarization of a short dielectric cylinder

Not so straight forward is the situation in the case of a short cylinder departing from the ellipsoidal shape, when exposed to an electric field (see Fig. 1).

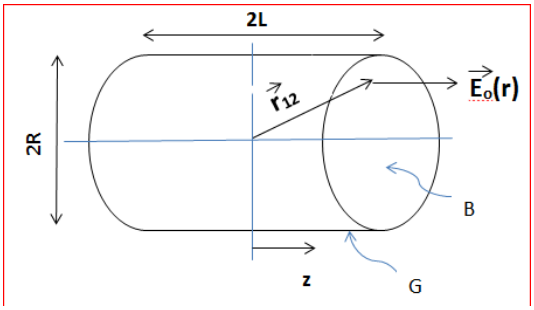

Fig.1.Dielectric cylinder of length *2L* and diameter *2R*. At B and G polarization charges accumulate

We find a homogeneous polarization in a first approximation step,

$$\vec{P}_1 = \frac{\varepsilon_0(\varepsilon - 1)\vec{E}_0}{1 + (\varepsilon - 1)\left(1 - (1 + R^2/L^2)^{-1/2}\right)}. \tag{5}$$

Due to the choice of the origin at z = 0, the by P generated field will be too weak in the transversal plane at z = 0, but along the z-axis at the limiting faces of the cylinder it is too strong. A further correction has to be made.
The dipole moment in a second approximation is given by

$$\vec{P} = \varepsilon_0(\varepsilon_p^* - \varepsilon_m^*)\vec{E}_0 \cdot \alpha = \varepsilon_0 \cdot K(\omega) \cdot \vec{E}_0 \tag{6}$$

with $K(\omega)$ the Clausius-Mossotti factor (CMF), and α the depolarization factor, and

$$\alpha = \left\{ \varepsilon_m^* + (\varepsilon_p^* - \varepsilon_m^*)\left[1 - (1 + R^2/L^2)^{-1/2} \right] \right\}^{-1} *$$

$$* \left\{ 1 + \frac{\frac{1}{2} - \left(1 + \frac{R^2}{L^2}\right)^{-\frac{1}{2}} - \frac{1}{2}\left(1 + \frac{8L^2}{R^2}\right)^{-1}}{(\varepsilon_p^* - \varepsilon_m^*)^{-1} + 1 - \frac{7}{16}\left(1 + \frac{11R^2}{56L^2}\right)} + \frac{\frac{1}{2L}\left(R^2 + 2L^2\right)\cdot\left(R^2 + 4L^2\right)^{-\frac{1}{2}} - \frac{1}{2L}R}{(\varepsilon_p^* - \varepsilon_m^*)^{-1} + 1 - \frac{7}{16}\left(1 + \frac{11R^2}{56L^2}\right)} \right\}.$$

We have taken into account that the dielectric cylinder of length *2L* and radius *R* displays a complex dielectric constant ε_p^* and is immersed in a suspending medium of a complex dielectric constant ε_m^* (see Zehe *et al.,* 2002). The CMF is a measure for the effective polarizability of the dielectric particle, and depends on the depolarization factor *α*, and thus very sensitively on the geometrical shape of the particle. The complex permittivity in its common expression is $\varepsilon^* = \varepsilon - j(\sigma/\varepsilon_0\omega)$, (*j*-imaginary unit), *σ* is the electrical conductivity of the dielectric medium. Given that in the case of a finite cylinder, as considered here, its length will be several times exceed the radius, we apply *f(q)*from Eq. (4), and arrive at a CMF of

$$K(\omega) = \frac{\varepsilon_p^* - \varepsilon_m^*}{\varepsilon_m^* + (\varepsilon_p^* - \varepsilon_m^*) \cdot f(q)} \tag{7}$$

In consequence, this factor depends, among other things, on the frequency of the applied electric field, and thus does the force acting on the particle. If only frequency dependencies are the objective of the study, it is sufficient to consider *K(ω)* and its dependence on particle properties and external field properties.

Electrorotation of a cylinder-shaped TMV bioparticle

A circularly polarized rotating electric field induces a rotating dipole moment in a dielectric object, which then will rotate in synchrony with the field, if the angular velocity of the field is not too large. Otherwise, the dipoles will lag behind the field. The time-averaged rotational torque in circularly polarized external fields, exerted on a particle, is given by the vector product of induced dipole moment and conjugate field,

$$< \vec{T} >= -\tfrac{1}{2}\,\mathrm{Im}[\vec{m}\, x\, \vec{E}^*]. \tag{8}$$

The induced dipole moment $\vec{m}$ is proportional to the external field *E*, the suspending medium permittivity ε_m^* and the volume *V* of the object. The torque is proportional to the imaginary component of the CMF and describes the frequency dependence of the rotation of an individual cell under study in or against the rotation sense of the external field. The minus sign indicates that the dipole moment lags behind the electric field. To determine the orientation of particle movement, only the directions (signs) of the torque components are needed. The sign of the torque about the vertical axis (z-axis) over the x-y plane, as considered in this paper, is equivalent to that of the frequency-dependent *K(ω)*-term:

$$sign<T_z>= sign\{Im[K^i(\omega)_x\text{-}K^i(\omega)_y]\} \tag{9}$$

Thus, if the imaginary component of $\vec{m}$ is positive, then the exerted torque will be negative and cause the particle to rotate in a sense that opposes that of the rotating field. We will consider the Tobacco Mosaic Virus (TMV) as specific bioparticle of cylindrical shape as treated in the foregoing sections, with properties given in Table 1. The TMV is immersed in an aqueous solution with ε_m and σ_m

Table 1. Properties of the TMV (subindex *p*), and of the aqueous solution (subindex *m*)

L	*2R*	ε_p	ε_m	σ_p	σ_m
25 nm	18 nm	55	78.5	0.085	0.001 S/m

Electrorotation spectra are displayed in Fig. 2, where the imaginary part of the CMF in dependence on the circular frequency ω of the electric field is shown. Each bell-shaped curve corresponds to a certain value of rod length L of the TMV. The maximum torque value occurs at frequencies around 10^6 rad/s, and is the larger the longer the TMV is chosen.

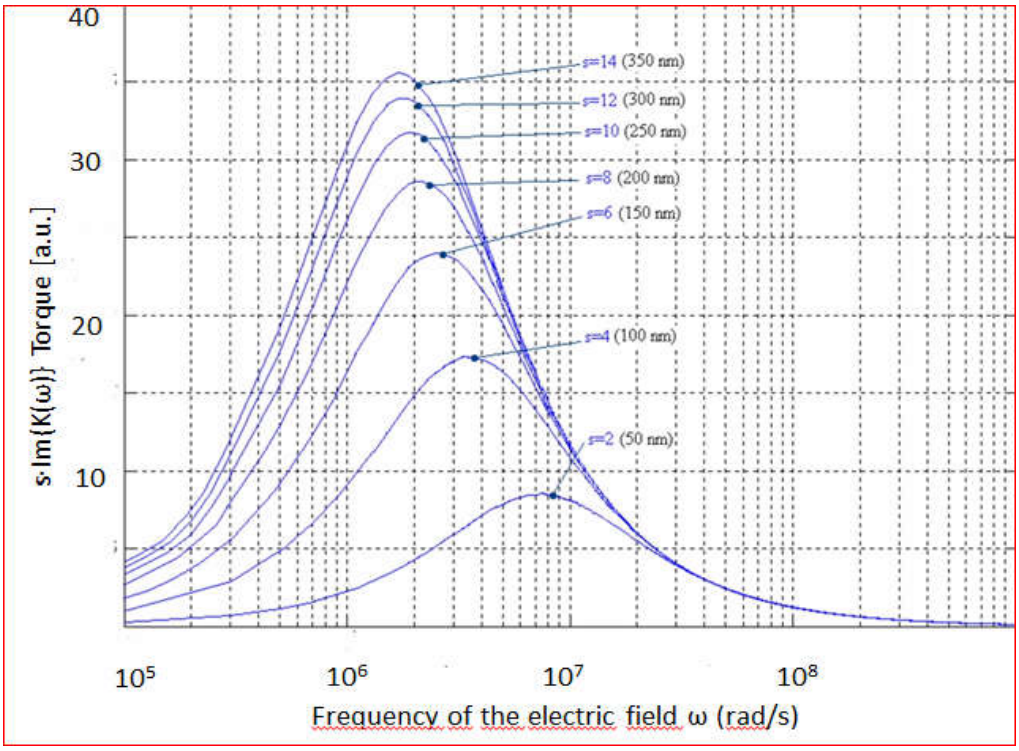

Fig. 2 Calculated electrorotational torque for different rod lengths of the TMV. With *s* a multiplication factor of the chosen minimum length of 25 nm is applied (*s* = 2, 4, 6, ...). The vertical axis displays a measure of the acting torque. Only the spectral range of positive torque is shown. The electrical conductivity of the medium used in the simulation is σ_m= 0.001 S/m.

Electrorotation-induced torque is easily controlled by altering the frequency of the electric field. Peak values depend on the rod size of the TMV with respect to the frequency position where the peak occurs, as well as the peak height, which is highest for the larger TMV rod. The fitting of theoretical electro-rotation spectra to experimentally determined data might require the consideration of hydrodynamic friction. The friction, experienced by the dielectric particle in the suspension medium affects the mobility in both electrorotation and dielectroforesis. Indeed, the counteracting frictional force will increase with TMV length (cell volume) too, and smaller rotation speeds are measured. Dismissing the Brownian movement and floating forces, the equation of movement is

$$\vec{p}\frac{du}{dt} = \vec{F}_{EK} - \vec{F}_{drag} \tag{10}$$

where $\vec{F}_{EK}$ is the electro rotation force.

The momentary angular velocity u is proportional to the instantaneous electro kinetic force

$$u = \vec{F}_{EK} / \vec{F}_f , \tag{11}$$

and substituting $\vec{F}_{EK}$ one gets

$$\vec{u} = \frac{V \cdot \varepsilon_0 \varepsilon_m^* Im[K(\omega)]\vec{E}_0^2}{2\vec{F}_f} , \tag{12}$$

with the friction force (η- viscosity of the medium, κ- friction coefficient),

$$\vec{F}_f = K\eta\vec{u} \quad . \tag{13}$$

Finally one arrives at a value for the rotation frequency W around a vertical axis of the cylindrical particle of length L (given that L>R),

$$W = \frac{\vec{u}}{L/2} \tag{14}$$

By altering the intensity of the acting electric field, E_0, the value of frequency $W[Hz]$ can be controlled. Considering a common quadrupole arrangement with a distance of 10 μm between opposite electrodes, then with the application of a voltage between 0…20 Volts, a range of altering the electric field up to $E_0=10^6$ V/m is reached. The rotation frequency W vs. the electric field strength E_0 for two different TMV length's L = 50nm and L = 300nm, respectively, is shown in Fig. 3.

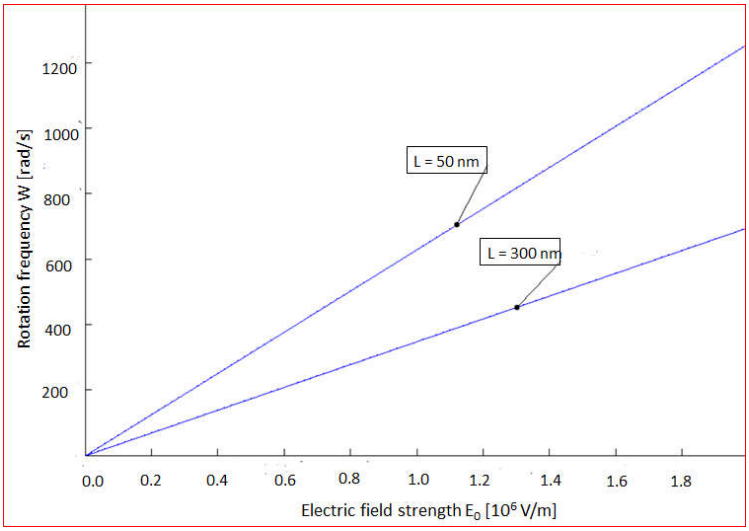

Fig. 3. The rotation frequency is expectantly higher for the shorter TMV rod and follows a linear proportionality to the applied electric field

Electrorotation was applied by Berg (2003)to drive the molecular motor of E-Coli bacteria. Speeds of up to 2,000 Hz were measured. Motor torque in either direction varied nearly linearly with speed up to over 100 Hz.

Summary

The approximation of particles of general shape as if they were ellipsoidal bodies is a frequently used approach in many theoretical studies. Advanced numerical methods consider the real size and shape of the particle in the electric field calculations, and these methods provide more accurate results than if an ellipsoidal approach is chosen. The Tobacco mosaic virus (TMV) has a rod-like geometry with an almost constant diameter of 18 nm along the cylinder axis. The presented results with realistic properties of the participating components prove that the electrorotation technique, applied to cylindrically shaped Tobacco Mosaic Virus (TMV) bioparticles of different lengths, provide for a rotative drive, controlled by the frequency of the electric field, and is suitable for the generation and control of movements in the way of a 'nano-propeller'.

Statement of competing interests
The authors declare no competing interests.

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