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Dynamic evolution of interacting carbon nanotubes suspended in a fluid using a dielectrophoretic framework

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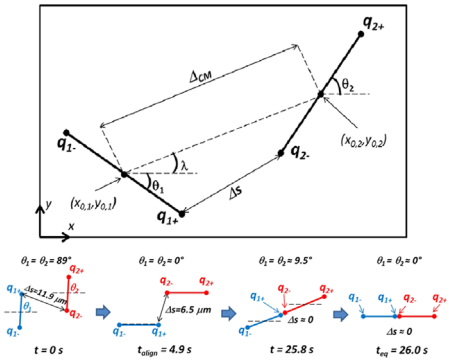
HIGHLIGHTS

- Two-dimensional motion of coupled CNTs under an AC electric field is investigated.
- Rotational and translational motion are modeled using coupled non-linear differential equations.
- High frequency, high solvent's polarity and long CNTs cause faster equilibrium.
- Experimental trends are adequately captured by the dielectrophoretic model proposed.
- Important insight into the underlying mechanisms of CNT manipulation is generated.

GRAPHICAL ABSTRACT



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ABSTRACT

A theoretical investigation of the dynamic response of interacting carbon nanotubes (CNTs) dispersed in a liquid medium under alternating current electric fields is presented. The proposed modeling strategy is based on the dielectrophoretic theory and classical electrodynamics of rigid bodies, and considers the coupled rotation-translation motion of interacting CNTs represented as electrical dipoles. Based on experimental evidence, the parameters which are expected to cause a major contribution to the CNTs' motion are investigated for different initial configurations of CNTs. It is predicted that high electric field frequencies, long CNTs, high values of electrical permittivity and conductivity of the CNTs immersed in solvents of high polarity promote faster equilibrium conditions, achieved by CNT tip-to-tip contact and alignment along the electric field direction. For the majority of the scenarios, CNT alignment along the field direction is predicted as the first event, followed by the translation of aligned CNTs until the tip-to-tip contact condition is reached. For systems with interacting CNTs with different lengths, equilibrium of the shorter CNT is achieved faster. Predictions also show that the initial rotation angles and initial location of CNTs have a paramount influence on the evolution of the system towards the equilibrium configuration.

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1. Introduction

The precise control and placement of carbon nanotubes (CNTs) are essential to achieve desired performance of novel devices at different scales. At small scales, alignment and manipulation of CNTs in liquids have shown great potential for the fabrication of nanoscale tips, fibrils, fibers, micro- and nano-electromechanical systems, among many others [1–3]. At larger scales, aligned CNTs are incorporated into thin films and bulk composites. It is well known that CNT-reinforced materials provide novel multifunctional performance for applications in several technological areas due to the extraordinary physical properties of the CNTs and the variety of the host materials available, being probably polymers and ceramics the most used ones [4]. To optimize the effective properties of such composite materials, different strategies to manipulate and/or align CNTs during fabrication have been developed. The aligned architectures aim to improve the effective properties of the materials in the direction of the CNTs due to their highly anisotropic properties [5–8]. Among such strategies, the application of electric fields emerges as one of the most convenient ones due to the electrical response of the CNTs and to its ease of implementation [9–12]. Depending on their quirality, singlewall carbon nanotubes (SWCNTs) have a semiconducting or metallic behavior, while multiwall carbon nanotubes (MWCNTs) are metallic as a consequence of the electronic interactions and transport among their walls [4,9]. The electrical response of the CNTs under electric fields can be thus investigated in terms of the polarization of the CNTs. For metallic CNTs, as their band gap is zero (or very small), polarizability along their length is dominant. On the other hand, due to their large band gap, the polarizability of semiconducting SWCNTs along their axis is comparable to the transverse polarizability and do not align along the electric field as metallic CNTs [13,14]. Thus, the response of CNTs to applied electric fields depends on the CNT type and on the electrical characteristics of the surrounding medium, among other factors. Due to the complex nature of the phenomenon, a clear understanding of the underlying mechanisms involved in the dynamics of CNTs immersed in liquid media under electric fields is still a scientific challenge; many efforts have been directed towards the exploration of such mechanisms. For example, An and Friedrich used a two-dimensional finite element simulation based on the effective dipole moment (EDM) approach from the dielectrophoretic (DEP) theory to predict the trajectory and time of assembly of a metallic CNT under an electric field [15]. They found that the assembly time depends on the distance between the CNTs and the electrodes and on the electric field magnitude. Ma and Guo used quantum mechanics calculations to investigate the mechanism of alignment of a SWCNT under an electric field by considering the dipole moment of the SWCNT [16]. They conclude that the rotational torque depends on the difference between longitudinal and transversal polarizabilities, with larger torques for longer CNTs. Monti et al. theoretically studied the rotation, translation and migration of CNTs towards an electrode under a direct current electric field by means of independent analytical expressions for each mechanism, comparing their outcomes to their experimental observations [17]. These authors reported that, compared to the translational time, the rotation contribution dominates the formation of CNT conductive networks. In a recent experimental and numerical work, Yang et al. highlight the importance of the CNT-to-CNT mutual interactions on the CNT dielectrophoretic assembly and concluded that factors such as CNTs' length and size of electrode gap play crucial roles on the final assembled configuration [18]. The effect of the electric field frequency on the rotational and translational motion of non-interacting CNTs has been previously investigated by a simplified one-dimensional framework, where the governing differential equations are non-coupled [19]. This uncoupled one-dimensional approach seems to adequate capture the major physics of the problem as well as, qualitatively, the major experimental trends, but is far from representing the actual phenomena occurring during experiments. Therefore, the current work contributes to a better understanding of the problem by considering the rotation and translation motion of two interacting (metallic) CNTs under an AC electric field, whose translation and rotation motion is governed by a set of coupled nonlinear differential equations. The dynamics of the chaining phenomenon between two interacting CNTs, considered as rigid dipoles, is explored in a two-dimensional framework by means of two-dimensional coupled rotational and translational governing equations. The coupling of such mechanisms stems from the Coulombic interactions between the CNTs due to the DEP induced charges. The set-up of the model resembles the experimental conditions previously investigated [12]. The current model is able to capture the influence of the dielectric properties of the suspending fluid, dissimilar length, electrical properties and initial conditions of the CNTs, on the dynamic evolution of the electric field-tailored CNT/liquid system.

2. Modeling strategy

2.1. Geometrical description and assumptions

The investigated system consists of two CNTs, labeled #1 and #2, with their centers of mass located at arbitrary positions defined by $\boldsymbol{r_1}$ and $\boldsymbol{r_2}$ and arbitrary orientational angles θ_1 and θ_2 defined with respect to the electric field ($\boldsymbol{E}$) direction (x-direction), as seen in Fig. 1. The system is modeled in two dimensions using a Cartesian x–y coordinate system. Based on the EDM approach from DEP theory [10,20–22], each metallic CNT is considered here as an electric dipole, modeled as a system of two electrical charges with identical magnitude and opposite signs, separated by a distance equal to the length of the CNT ($2a$, with a as the CNT major semiaxis), and concentrated at the CNT's ends, see Fig. 1. It is also assumed that the dipole induced on the CNTs follows the direction of the electric field and, as a consequence, the positive charge of the CNTs will always stand to the right of the negative charge. In Fig. 1 $\boldsymbol{r_1}$ and $\boldsymbol{r_2}$ indicate the positions of the centers of mass of CNTs 1 and 2 and are described by the coordinates (x_1,y_1) and (x_2,y_2). The angle θ_i ($i=1,2$) is the angle between the longitudinal axis of the CNT and the direction of the electric field (x-direction), and its value range from $-\pi/2$ to $\pi/2$. CNTs are deemed oriented along the direction of the electric field when $\theta_i=0$ and positive values of θ_i correspond to the situation where the CNT's positive charge is located above the position of the center of mass of the CNT, as for the case of "CNT-2" in Fig. 1.

The position vectors for the positive ($\boldsymbol{r_i}^+$) and negative ($\boldsymbol{r_i}^-$)

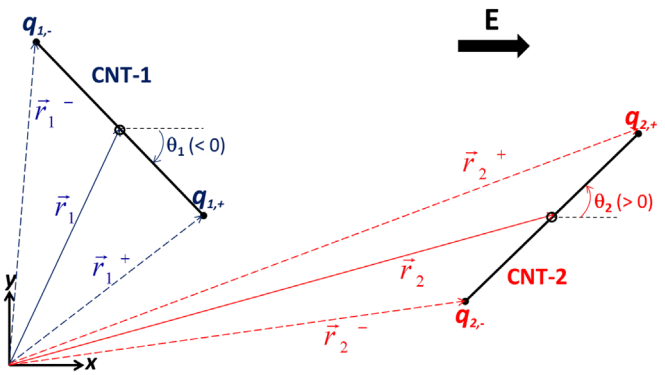

Fig. 1. Schematic of the modeled system containing two interacting CNTs.