Alignment dynamics of single-wall carbon nanotubes under electric field in different surfactant solutions

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Abstract

The dynamics of metallic single-wall carbon nanotube (SWCNT) alignment inside various viscous media under electric field is investigated in this simulation work for the manifestation of macroscale aligned SWCNT films. An alternating current (AC) electric field was applied to the liquid solution of several surfactants (DIW, DMF, CHEX, SDS, and DOC) containing SWCNTs. The time required for the SWCNTs to get aligned to the applied AC electric field was simulated for different initial conditions for all the surfactants. An analytical model based on dielectrophoresis induced torque was employed. The model considers the viscosity and conductivity of the surrounding medium. The influence of SWCNT length, SWCNT radius, and frequency of the AC field on the assembly of SWCNTs were studied. Our analysis showed that a longer and narrower SWCNT prompts faster assembly to an aligned SWCNT aggregation. Furthermore, the effect of the concentration of SDS and the effect of electric field strength for DIW surfactant were also investigated. Viscosity plays a significant role in the alignment process. Slower SWCNT alignment is caused by a medium of higher viscosity.

1. Introduction

Carbon nanotubes can be two types based on the number of the wall; single-wall carbon nanotube (SWCNT), that can be demonstrated as a single layer graphene rolled up to cylinder, and multi-wall carbon nanotube (MWCNT), that can be illustrated as cylinders of multiple graphitic sheets. MWCNTs have mainly metallic behavior as a result of electronic interaction and transport among their walls and hence show conductivity similar to copper, whereas the conductivity of SWCNT depends on chirality [1, 2]. SWCNTs have some phenomenal electrical, optical, and thermal properties which can be exploited in diverse applications. They exhibit strong optical absorption and emission due to the van Hove singularities in the density of states that come from their 1D nature [3]. Photoluminescence and electroluminescence result in due to the radiative recombination of excitons and electron-hole pairs, respectively, which can be created electrically and optically [4, 5]. Therefore, SWCNTs show great promises for optoelectronic and thermal applications. Promising applications of CNTs include terahertz (THz) light emitter [6], infrared emitter [7], single-photon emitter [8], ultra-broadband thermal light emitter [9], thermoelectronic devices [10–12], THz polarizers [13], wearable technologies [14], supercapacitor [15], nanocomposites [16–19], thermal interfaces [20, 21], and many others.

For most applications, CNTs are required to be deposited on substrates in a specific pattern like horizontal or vertical relative to the substrate so that it results in a periodic aligned pattern. However, despite considerable efforts to develop ways to produce microscale architectures of aligned nanotubes, macroscopic manifestations of aligned nanotubes are limited. The purpose of the aligned architectures is to enhance the materials’ effective properties in the direction of the axis of CNTs as their properties are highly anisotropic [22–24]. Such architecture facilitates rapid carrier transport, high thermal and electrical conductivity, high stability, long life cycle, high structural uniformity, high optical absorption, and high mechanical strength [24, 25].
mechanical, and magnetic techniques have been investigated for the alignment of CNTs in polymers and other viscous media. Besides, direct manipulation of individual CNT with atomic force microscopy has been investigated [26]. Despite promising results obtained in mechanical [27, 28] and magnetic [29, 30] techniques for CNT alignment, structural damage caused by a mechanical process, and the need for a very high magnetic field are the major drawbacks of these techniques. Due to the high cost, complex, and time-consuming nature, direct manipulation of individual CNT with atomic force microscopy is not suitable for mass-scale assembly of CNTs [26]. Hence, the electrical technique emerges as a viable option for CNT alignment in viscous media.

Utilizing an alternating current (AC) field is effective for the alignment of SWCNTs in the solution that results from the dielectrophoresis (DEP) effect [31]. In dielectrophoresis (DEP), a non-uniform electric field is used to induce a dipole moment in a suspended particle. The particle moves towards or away from the high electric field, depending on the suspending medium. If the polarization of the particle surpasses the polarization of the suspending medium, the particle moves towards the region of higher field strength (positive DEP); whereas, if the polarization of the suspending medium surpasses the polarization of the particle, the particle moves towards the low potential area (negative DEP). DEP is gaining popularity in microscale device construction in recent years, and one of the main reasons is the decrease in electrode spacing as it allows higher effective field strengths [32]. As the bandgap for metallic CNTs is zero or very small, polarizability along their length is dominant, whereas, due to the large bandgap in semiconducting CNTs, polarizability along the axis is comparable to the transverse polarizability. As a result, semiconducting CNTs do not align well along the electric field compared to metallic CNTs [33]. Therefore, CNT type and electrical properties of the surrounding medium, along with other factors, determine the response of CNT to the applied electric field.

Here, we studied the alignment dynamics of SWCNTs in five different viscous media using the DEP effect in the presence of an AC electric field. The surfactants used here are deionized water (DIW), sodium dodecyl sulfate
(SDS), sodium deoxycholate (NaDOC), cyclohexane (CHEX), and dimethylformamide (DMF). Alignment time for different initial conditions, the effect of change in SWCNT length, the effect of change in SWCNT radius, the effect of change in electric field frequency were extensively studied in this work. Moreover, the effect of variation in concentration for SDS surfactant and the effect of electric field strength variation for DIW surfactant were investigated. Furthermore, we developed an empirical equation of alignment time dependence on SWCNT length, SWCNT radius, electric field frequency, and SDS concentration for SDS surfactant. As the surfactants studied here are widely used for SWCNT dispersion, this study will help in a better understanding and designing of the alignment process.

2. Methods

2.1. Analytical modeling

To understand the dynamics of SWCNT alignment in presence of an AC electric field in a viscous medium, an analytical model considering the dielectrophoresis induced torque [34, 35] and the viscous effect of the surrounding medium was used. A representative SWCNT used in this study is shown in figure 1. The illustration of the setup for applying the AC electric field is shown in figure 2. The time required for SWCNT alignment along the electric field direction was predicted by solving the rotational motion equation. Using Newton’s second law of motion, the governing equation of the rotational motion of a cylindrical SWCNT immersed in a viscous medium in the presence of an external AC electric field is given by [36],

$$I\frac{d^2\theta}{dt^2} + \tau_\eta + \tau_{\text{align}} = 0.$$  

Here, $I$ is the moment of inertia of the SWCNT, $\theta$ is the angular position of the SWCNT axis with respect to the direction of the AC electric field, $\frac{d^2\theta}{dt^2}$ is the second derivative of $\theta$ with respect to time $t$, $\tau_\eta$ is the damping torque and $\tau_{\text{align}}$ is the SWCNT dielectrophoretic-induced torque. The expressions for damping torque, $\tau_\eta$ is given by [34],

$$\tau_\eta = 8\pi\eta\Omega \frac{d\theta}{dt},$$

where $\eta$ is the viscosity of the medium, and $\Omega$ is the volume of the SWCNT. The expressions for dielectrophoretic-induced torque, $\tau_{\text{align}}$ is given by,

$$\tau_{\text{align}} = \frac{1}{4}\Omega \varepsilon_m \text{Re}[\alpha^*] E^2 \sin 2\theta.$$  

In equation (3), $\varepsilon_m$ is the permittivity of the medium surrounding the SWCNT, $E$ is the magnitude of the applied electric field, Re denotes the real part of the complex expression within brackets and $\alpha^*$ is a complex term which is given by,

$$\alpha^* = \frac{(\varepsilon^*_m - \varepsilon^*_\text{CNT})^2}{[\varepsilon^*_m + (\varepsilon^*_\text{CNT} - \varepsilon^*_m)D](\varepsilon^*_\text{CNT} + \varepsilon^*_m)}.$$
\[ \epsilon_{m,CNT}^* = \epsilon_{m,CNT} - j \frac{\sigma_{m,CNT}}{\omega}. \]  

In above equations, \( \epsilon_{m}^* \) and \( \epsilon_{CNT}^* \) are complex numbers expressed in terms of the electrical permittivities \( \epsilon \) and conductivities \( \sigma \) of the medium (\( m \)) and SWCNT (\( CNT \)) respectively, where \( m = \text{DIW}, \text{SDS}, \text{NaDOC}, \text{CHEX}, \text{DMF} \). \( \omega \) is the angular frequency of the applied field (\( \omega = 2\pi f \)). The depolarization effect, \( D \) is given by [37],

\[ D \approx \left( 4r_0^2 / \pi^2 \right) \left[ \ln(1/\eta) - 1 \right]. \]  

Equation (1) is a second-order nonlinear damped differential equation as \( \tau_q \) depends on \( \frac{d\theta}{dt} \) and \( \tau_{align} \) depends on \( \sin 2\theta \). Frequency of the applied electric field \( f = \omega / 2\pi \), permittivities, and conductivities are other control parameters. The dynamic alignment of SWCNTs, represented by the angle \( \theta \) between the major axis of the SWCNT and the electric field direction, is found by solving equation (1). \( \theta(t = 0) = \theta_0 \) is the initial angular position of the SWCNT and for aligned SWCNT \( \theta = 0^\circ \). From this, time required for such an alignment condition can be estimated. By considering an SWCNT as a highly elongated cylinder, the time for SWCNT alignment was calculated for different surrounding media such as DIW, SDS, NaDOC, CHEX & DMF. The volume \( \Omega \) and the moment of inertia \( l \) of the SWCNT were taken as \( \Omega = \pi (r_o^2 - r_i^2)l \) and \( l = (1/12)M^2l^2 \) where \( r_o, r_i, l \) and \( M \) are the outer radius, inner radius, length and mass of the SWCNT respectively. The differential equation in (1) was solved using Runge-Kutta 4th order method. Runge-Kutta method is derived from an appropriate Taylor method in such a way that the Final Global Error (FGE) is of \( O(h^5) \). As the Runge-Kutta method of order \( N = 4 \) is most popular for its accuracy, stability, and ease of implementation, we used this method. MATLAB was used for the simulation. The solution of equation (1), \( \theta(t) \) gives us the dynamic evolution of the SWCNT position i.e., the angle between the axis of SWCNT and the applied electric field.

### 2.2. Simulation parameters

The values used for SWCNT electrical permittivity and conductivity were \( \epsilon_{CNT} = 2000\epsilon_0 \) and \( \sigma_{CNT} = 1 \times 10^{-3} \) Sm \(^{-1} \) respectively, \( \epsilon_0 \) is the permittivity of the free space \( \epsilon_0 = 8.854 \times 10^{-12} \) Fm \(^{-1} \). The electric field magnitude used was \( E = 6.6 \) kV m \(^{-1} \).

The conductivity of DIW, \( \sigma_{DIW} = 5.5 \times 10^{-6} \) Sm \(^{-1} \), dielectric constant, \( \epsilon_{DIW} = 80\epsilon_0 \), medium viscosity, \( \eta_{DIW} = 1 \times 10^{-3} \) Pa s [38]. While investigating the effect of SWCNT length, the length was varied from 3 \( \mu \)m to 10 \( \mu \)m. The radius of SWCNT was varied from 0.5 nm to 3 nm for investigating the effect of radius on alignment time. The frequency was swept from 1 Hz to 300 kHz, and finally, the electric field was stretched from 2.6 kV m \(^{-1} \) to 10.6 kV m \(^{-1} \) for this surfactant.

For SDS surfactant, medium conductivity, \( \sigma_{SDS} = 8 \times 10^{-3} \) Sm \(^{-1} \) for concentration of 0.8 \( \times 10^{-3} \) mol L \(^{-1} \) [39], dielectric constant, \( \epsilon_{SDS} = 58\epsilon_0 \) and medium viscosity, \( \eta_{SDS} = 1 \times 10^{-3} \) Pa s. SWCNT length was varied from 1 \( \mu \)m to 10 \( \mu \)m were used for determining the effect of SWCNT length on alignment time. Radius was varied from 0.5 nm to 3 nm. The frequency was swept from 100 Hz to 5 MHz. The concentration of SDS was varied from 0.87 mmol L \(^{-1} \) to 38 mmol L \(^{-1} \).

For NaDOC surfactant, medium conductivity, \( \sigma_{NaDOC} = 1 \times 10^{-6} \) Sm \(^{-1} \), dielectric constant, \( \epsilon_{NaDOC} = 4.7\epsilon_0 \) and medium viscosity, \( \eta_{NaDOC} = 1.958 \times 10^{-3} \) Pa s [40]. For NaDOC surfactant, SWCNT length was varied from 78 \( \mu \)m to 20 \( \mu \)m. Radius was varied from 0.5 nm to 2.5 nm. The frequency was swept from 100 Hz to 3 MHz.

For CHEX surfactant, medium conductivity, \( \sigma_{CHEX} = 0 \) Sm \(^{-1} \), dielectric constant, \( \epsilon_{CHEX} = 2\epsilon_0 \) and medium viscosity, \( \eta_{CHEX} = 0.29 \times 10^{-3} \) Pa s [38]. SWCNT length was stretched from 6 \( \mu \)m to 18 \( \mu \)m for CHEX surfactant. Radius was varied from 0.5 nm to 2.5 nm. The frequency was swept from 100 kHz to 7 MHz.

For DMF surfactant, medium conductivity, \( \sigma_{DMF} = 15.9 \times 10^{-6} \) Sm \(^{-1} \), dielectric constant, \( \epsilon_{DMF} = 38\epsilon_0 \) and medium viscosity, \( \eta_{DMF} = 0.92 \times 10^{-3} \) Pa s [38]. In this surfactant, SWCNT length ranged from 6 \( \mu \)m to 18 \( \mu \)m. Radius ranged from 0.5 nm to 2.5 nm. The frequency was swept from 100 Hz to 500 kHz.

### 3. Results and discussion

Structure of SWCNTs and properties of solution contribute significantly to the alignment dynamics of SWCNTs. The viscosity, conductivity, permittivity, and concentration are the determining parameters of the surrounding medium. Here, the effect of initial angular position, SWCNT length, SWCNT radius, and electric field frequency were studied for various surfactants. The effect of concentration of SDS and the effect of electric field strength for DIW surfactant were also investigated. The alignment time was calculated from the simulation graph. The alignment time, \( \tau_{align} \) is defined as the time required for \( \theta(t) \) reduced to zero or simply as the time required for the SWCNTs to get aligned with the applied electric field.
Figure 3. Angular Position of SWCNT as a function of time for different initial angles for DIW solvent.

Figure 4. Angular Position of SWCNT as a function of time for different initial angles for SDS surfactant.

Figure 5. Angular Position of SWCNT as a function of time for different initial angles for NaDOC surfactant.
3.1. Impact of surfactant and initial angular position of SWCNT

We analyzed the effect of the initial angular position. SWCNT length of 10 $\mu$m, electric field frequency of 10 kHz, SWCNT radius of 1 nm were considered. Three different initial conditions were investigated: 89°, 60°, and 30° (89° was taken instead of 90° to avoid undefined numeric condition). The less the initial angular position the less time the SWCNT takes for alignment.

DIW was used as the first surfactant. SWCNT length, SWCNT radius, and electric field frequency were used as mentioned earlier. In figure 3, 89°, 60°, and 30° initial angular position conditions are shown for DIW surfactant in blue dashed line, red dash-dotted line, and solid green line, respectively. Alignment times were 0.36 ms, 0.20 ms, and 0.18 ms for 89°, 60°, and 30°, respectively. With the decrease in initial angle, the time required for alignment decreases as less rotation is required for alignment.

The second surfactant used here was SDS. Alignment time of 0.9 ms, 0.5 ms, and 0.4 ms was found for initial angular position of 89°, 60°, and 30°, respectively. In figure 4, 89°, 60°, and 30° initial conditions are shown in blue dashed line, red dash-dotted line, and solid green line, respectively.

For NaDOC surfactant, alignment time of 12 ms, 7 ms, and 5 ms were found for initial angular position of 89°, 60°, and 30°, respectively, and figure 5 represents them in blue dashed line, red dash-dotted line, and solid green line accordingly.

For CHEX surfactant, in figure 6, 89°, 60°, and 30° initial angular conditions are shown in blue dashed line, red dash-dotted line, and green solid line and alignment time of 4.1 ms, 2.2 ms, and 2 ms were found for them respectively.
For DMF surfactant, alignment time of 0.7 ms, 0.4 ms, and 0.3 ms was found for an initial angular position of 89°, 60°, and 30°, and they are presented in figure 7 using blue dashed line, red dash-dotted line, and solid green line respectively.

**Table 1.** Alignment time for different initial conditions for different surfactants.

| Name of surfactant | Alignment time (ms) |  
|--------------------|---------------------|  
|                    | For 89°  | For 60°  | For 30°  |  
| DIW                | 0.36     | 0.20     | 0.18     |  
| SDS                | 0.90     | 0.50     | 0.40     |  
| NaDOC              | 12       | 7        | 5        |  
| CHEX               | 4.10     | 2.20     | 2.00     |  
| DMF                | 0.70     | 0.40     | 0.30     |  

For DMF surfactant, alignment time of 0.7 ms, 0.4 ms, and 0.3 ms was found for an initial angular position of 89°, 60°, and 30°, and they are presented in figure 7 using blue dashed line, red dash-dotted line, and solid green line respectively.
A comprehensive study of initial angular position variation for all the five surfactants is represented in figure 8. The blue bar, orange bar, and grey bar represent an initial angle of $89^\circ$, $60^\circ$, and $30^\circ$ respectively in each case.
The time required for alignment in each case is presented in table 1. We can see that it took the longest for NaDOC surfactant and fastest for DIW surfactant.

3.2. Effect of length

The effect of different lengths of SWCNT is calculated. Here, an initial angular position of 89°, an electric field frequency of 10 kHz, SWCNT radius of 1 nm was considered. With the increase in SWCNT length, alignment time decreases. The dielectrophoresis (DEP) induced torque strongly depends on the SWCNT length. Castellano et al [23] reported that the degree of alignment of SWCNTs is dependent on the SWCNT length. Although, the damping torque also depends on SWCNT length, the influence of SWCNT length on DEP induced torque is much stronger for longer SWCNTs. Moreover, it can be mathematically deduced from equations (3), (4), and (6) that induced torque has higher order proportional dependency on SWCNT length compared to damping torque. As the DEP induced torque is much larger for longer SWCNTs, they tend to align faster.

From figure 9, it is eminent that with increasing length, the alignment time decreases. As the length increases, the dipoles at the tips of SWCNTs respond faster to the electric field, and thus the alignment time is reduced. Alignment time of 3.5 ms, 2 ms, 1.3 ms, 1 ms, 0.65 ms, and 0.45 ms was found for SWCNT lengths of 3 μm, 4 μm, 5 μm, 6 μm, 8 μm, and 10 μm respectively and they are represented in figure 9(a) as blue dash-dotted line, red dotted line, green dashed line, cyan dash-dotted line, solid magenta line and black dashed line respectively. Another graphical measurement of the alignment time is given as a function of SWCNT length in figure 9(b).

Similar to the previous surfactant, the alignment time decreases with the increase in length for SDS surfactant too. In figure 10(a), blue dash-dotted line, red dotted line, green dashed line, cyan dash-dotted line, magenta dashed line, and black dashed line represent the case for SWCNT with the length of 1 μm, 1.5 μm, 2 μm, 3 μm, 5 μm and 10 μm respectively and alignment time of 4.5 ms, 2.5 ms, 1.8 ms, 1.4 ms, 1 ms, and 0.9 ms were observed accordingly. Alignment time versus SWCNT length of the SWCNT curve is given in figure 10(b).

Effect of SWCNT length on alignment time for NaDOC and CHEX surfactants can be found in the supplementary material1 available at stacks.iop.org/MRX/8/045609/mmedia.

3.3. Effect of radius

The variation of SWCNT diameter or radius has a significant effect on alignment time. Here SWCNT length of 10 μm and frequency of 10 kHz was set. The narrower it gets, the less time is required for SWCNT alignment.

\[ t_{\text{align}} = a e^{bl} + c e^{dl} \text{ ms}, \]

where, \( a = 21.24, b = -1.925, c = 1.471, \) and \( d = -0.05405 \) are empirical parameters.

We also measured the variation of length for the DMF surfactant. The effect is shown in figure 11(a) as blue dash-dotted line, red dotted line, green dashed line, solid cyan line, magenta dotted line, and black dashed line for SWCNT length of 6 μm, 8 μm, 10 μm, 12 μm, 15 μm and 18 μm, respectively and alignment time of 1.70 ms, 1.15 ms, 0.70 ms, 0.55 ms, 0.35 ms, and 0.30 ms were found. The relation between alignment time and length of the SWCNT curve is represented in figure 11(b).

Effect of SWCNT length on alignment time for NaDOC and CHEX surfactants can be found in the supplementary material1 available at stacks.iop.org/MRX/8/045609/mmedia.

1 See supplemental material at stacks.iop.org/MRX/8/045609/mmedia for effect of CNT length, radius, and frequency on alignment dynamics for NaDOC and CHEX., 2021.
Representation of SWCNTs having different radius is shown in figure 12. For narrower SWCNTs, depolarization factor decreases which in turn increases the DEP induced torque. Moreover, this can be mathematically corroborated from equations (3), (4), and (6). Therefore, narrower SWCNTs tend to align faster and shorter time were required.

Figure 13. For DIW solvent, (a) effect of radius on alignment time, and (b) alignment time of SWCNT as a function of SWCNT radius.

Figure 14. For SDS surfactant, (a) effect of variation of radius of SWCNT, and (b) alignment time of SWCNT as a function of SWCNT radius.
For the radius of 0.5 nm, 1 nm, 1.5 nm, 2 nm, 2.5 nm, and 3 nm, alignment times were found 0.2 ms, 0.4 ms, 0.7 ms, 1.1 ms, 1.6 ms, and 2.2 ms, respectively for DIW surfactant. In figure 13(a) blue dash-dotted line, red dotted line, green dashed line, solid cyan line, magenta dotted line, and black dashed line represent the cases for
0.5 nm, 1 nm, 1.5 nm, 2 nm, 2.5 nm and 3 nm, respectively. The relation of alignment time with radius is shown in figure 13(b).

Next we studied the effect of the SWCNT radius on the alignment time for the SDS surfactant. With the increase of SWCNT radius, alignment time also increased. Alignment times of 0.90 ms, 0.95 ms, 1.00 ms, 1.05 ms, 1.12 ms, and 1.20 ms were found for SWCNT radius of 0.5 nm, 1 nm, 1.5 nm, 2 nm, 2.5 nm, and 3 nm, respectively. In figure 14(a) blue dash-dotted line, red dash-dotted line, green dashed line, cyan dotted line, magenta solid line, and black dotted line represent the case for SWCNT radius of 0.5 nm, 1 nm, 1.5 nm, 2 nm, 2.5 nm, and 3 nm, respectively. The relation of alignment time with radius is shown in figure 14(b). An empirical equation for the alignment time with SWCNT radius was developed here by curve fitting of second order polynomial. The empirical equation was found as

$$t_{\text{align}} = 0.016429 r^2 + 0.060 214 r + 0.869$$ \text{ms.} \quad (8)$$

The effect of radius variation for DMF surfactant can be found from the figure 15(a). Blue dashed line, red dashed line, green dash-dotted line, cyan dash-dotted line, and magenta solid line were used for SWCNT radius of 0.5 nm, 1 nm, 1.5 nm, 2 nm, and 2.5 nm, respectively. Alignment times varied from 3 ms to 0.3 ms for radius variation of 2.5 nm to 0.5 nm. Alignment time as a function of SWCNT radius is shown in figure 15(b).

Effect of SWCNT radius on alignment time for NaDOC and CHEX surfactants can be found in the supplementary material (see footnote 1).

3.4. Effect of variation in frequency

The impact of the variation in the AC electric field frequency on the alignment time was also studied. Here the SWCNT length and radius was taken as 10 μm, and 1 nm, respectively. Beyond a certain frequency, the alignment time increases, and up to that frequency, alignment time remains almost constant.

For DIW surfactant, alignment time remains almost constant for frequency up to 1 kHz. Beyond that, with the increase in frequency, alignment time also increases. This is due to the fact that the SWCNT does not get sufficient time to respond due to the high electric field frequency. For frequency up to 1 kHz, alignment time was 0.7 ms. For a frequency of 10 kHz and 300 kHz, alignment times of 0.9 ms and 2.2 ms were found, respectively. In figure 16(a), blue dashed line, red dashed line, green dash-dotted line, cyan dash-dotted line, solid magenta line, and black dotted line represent the case of electric field frequency of 1 Hz, 10 Hz, 100 Hz, 1 kHz, 10 kHz, and 300 kHz respectively. The relation of alignment time with electrical field frequency is shown in figure 16(b).
Next the effect of frequency on the alignment time was simulated for SDS surfactant. For frequency up to 10 kHz, alignment time was almost constant, which is 1 ms. Alignment times of 1.2 ms, 1.5 ms, 2.2 ms, and 4.2 ms were found for a frequency of 1 MHz, 2 MHz, 3 MHz, and 5 MHz, respectively. In figure 17(a) blue
dashed line, red dashed line, green dash-dotted line, cyan dash-dotted line, magenta dotted line, and solid black line represent the cases for electric field frequency of 100 Hz, 10 kHz, 1 MHz, 2 MHz, 3 MHz, and 5 MHz, respectively. The relation of alignment time with electric field frequency is shown in figure 17 (b). By curve fitting of second order polynomial, an empirical equation was found for the alignment time with the field frequency variation and it was found as,

\[ t_{\text{align}} = 1.2307 \times 10^{-13} f^2 + 2.3115 \times 10^{-08} f + 1.0076 \text{ ms}. \] (9)

The effect of frequency was also observed for DMF surfactant. For frequency up to 100 kHz, alignment time was almost constant, which is 0.9 ms. Alignment times of 0.95 ms, 2 ms, and 4 ms were found for a frequency of 100 kHz, 300 kHz, and 500 kHz, respectively. In figure 18(a) blue dashed line, red dashed line, green dash-dotted line and magenta dotted line represent the cases for electric field frequency of 100 Hz, 10 kHz, 100 kHz, 300 kHz, and 500 kHz. The relation of alignment time with electric field frequency is shown in figure 18(b).

Effect of frequency variation on alignment time for NaDOC and CHEX surfactants can be found in the supplementary material (see footnote 1).

3.5. Variation of concentration
We also investigated the variation of concentration for SDS surfactant. For the cases mentioned up to this, SDS concentration was considered as 0.8 mmolL\(^{-1}\). In the case of variation of concentration of SDS surfactant, SWCNT length of 1 \( \mu \)m, SWCNT radius of 1 nm, and frequency of 10 kHz, were considered.

With an increase in concentration, conductivity and viscosity increase, and with that, the alignment time also increases. Alignment times of 1 ms, 1.6 ms, 2.7 ms, 3.1 ms, 4.9 ms, and 6 ms were found for a concentration of 0.87 mmol L\(^{-1}\), 1.74 mmol L\(^{-1}\), 3.47 mmol L\(^{-1}\), 4.34 mmol L\(^{-1}\), 6.94 mmol L\(^{-1}\), and 8.68 mmol L\(^{-1}\), respectively and they are represented in figure 19(a). Electrical conductivity and permittivity of SDS were collected from literature [39]. Alignment time with respect to concentration is shown in figure 19(b). The relation between alignment time and SDS concentration was found as an empirical equation using linear curve fitting as,

\[ t_{\text{align}} = 0.63785 C_{\text{SDS}} + 0.44841 \text{ ms}, \] (10)

where \( C_{\text{SDS}} \) denotes the SDS concentration.
3.6. Variation of field strength

Finally, the effect of field strength on alignment time was investigated for the DIW surfactant. Here SWCNT length of 10 μm, SWCNT radius of 1 nm, and field frequency of 10 kHz were used. As the AC electric field strength increases, alignment time decreases, which means SWCNTs tend to align faster. For field strength of 2.6 kV m⁻¹, 4.6 kV m⁻¹, 6.6 kV m⁻¹, 8.6 kV m⁻¹, and 10.6 kV m⁻¹ alignment time were found as 2.5 ms, 0.75 ms, 0.45 ms, 0.20 ms, and 0.15 ms, respectively and were shown in figure 20(a). The relation of alignment time with electric field strength is given in figure 20(b).

4. Conclusion

The alignment process of the SWCNT network in five different viscous media under the application of an AC electric field using an analytical model that considers dielectrophoretic torque and the viscous effect of the surrounding medium was explored. The initial angular position of the SWCNTs with the applied electric field, SWCNT length, SWCNT radius, frequency of the applied electric field, conductivity and permittivity, and the viscosity of the medium play the governing role in the alignment process. The lower the initial angular position, the lower time is required for alignment. For larger SWCNTs, less time is required for the alignment process as larger SWCNTs have larger dipole induced. Similarly, less time is required for the alignment process for narrower SWCNTs. As the diameter of SWCNTs increases, more time is required. Therefore, longer and narrower SWCNTs tend to align faster. Among the various factors on which the alignment time of SWCNTs depend on, in our opinion, viscosity is the most significant factor. Change in alignment time due to CNT length, CNT radius or electric field frequency is not as drastic as change in alignment time owing to the viscosity of the surfactant. Damping torque increases (decreases) significantly with the increase (decrease) in viscosity of the medium. Viscosity significantly contributes to the alignment time of SWCNTs, as damping torque counteracts DEP induced torque. Our simulation results also reflect the pronounced dependence of alignment time on viscosity e.g., the highest alignment time was found for SWCNTs in NaDOC surfactant which has the highest viscosity.

In this work, the factors, that contribute to the agility of SWCNT alignment, were manipulated and the simulation results were reported. The outcome of this study will help a better understanding of the fabrication of macroscale aligned SWCNT films and CNT based composite nanostructures, which will be paramount for diverse electronic, optoelectronic, photonic, and thermal applications.

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