Handling the volume density of Carbon nano tube membranes: experiment and particle based simulation

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Abstract: In forests and membranes, Carbon nano tubes (CNT) are not individualised, instead they tend to be agglomerated into bundles because of the strong van der Waals interaction [1]. CNTs usually form into bundles containing up to hundreds or thousands of parallel CNTs named as fibres which create networks within a CNT membrane. Recently, CNT based macrostructures (yarn and membrane) have increasingly been used in various applications in electronics, medical and bioengineering. Meanwhile the volume density of CNTs impacts on mechanical and physical properties of macrostructures, the handling of the density of membranes is very complex. Thus, in this paper, an electric processing to dilate CNT membrane is sufficiently studied and investigated by both the experiment and particle based numerical simulation. Several potential applications of the method are also represented not only to handle the density of CNTs but also to improve the CNTs' alignment in macro-structures.

1. Formation and model of CNT membranes

The CNT macrostructures including yarns and membranes start by forming web, whereby a forest of vertically oriented CNT forest is converted to a horizontally continuous web. CNT fibres are oriented along the web axis in a variety of ways, some of them are parallel and others are poorly aligned or coiled [2]–[5] (Fig.1). Since the CNT web impacts on the properties of derived macrostructures, the simulation of CNT membranes has attracted significant attentions [5]–[7]. For example, a model by Kunznetsov and his co-workers [5] proposed that the connection between CNT fibres is the basis for the continuous spinning of CNT web and then yarn from CNT forests. Such models postulate that the densification effect at the top and bottom of the forest strengthens the fibres interconnections when being pulled out a CNT wafer. However, the scanning electron microscopy (SEM) analysis of CNT webs showed that CNT fibres entang le together. This entanglement is a key factor for the formation of CNT macrostructures because it allows the array of parallel fibres to unfold continuously into a

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CNT matrix. The entanglement of CNT fibres can be regarded as networks made of fibres' entanglement junctions (Fig. 2) [3], which have a strong relation with the properties of derived CNT macrostructures We reckon that CNT fibres are movable because the constraint imposed by the surrounding CNTs can change due to their own motion and a constraint will disappear if surrounding CNTs shift. Thus, the entanglement of CNT membrane (or fibres) can be modelled using the dual slip-link theory which was introduced by Doi and Takimoto [8] in modelling polymeric materials. For this model, the entanglement junction is represented by a slip link through which fibre chains can pass freely. The CNT fibres are linked together by slip links which are destroyed if fibres slide off slip links. This model corresponds to the formation of a random network of CNT fibres with non-uniform tension pulled out of a CNT forest. Owing to such structure, CNT membrane can be flexible by a load. Over the last two decades, CNT membrane has increasingly been used in various applications of electronics, medical and bioengineering [9],[10]. While the density of CNTs impacts on mechanical and physical properties of CNT membranes, the processing of CNT membrane density is interesting but very challenging.

Besides aligning CNTs in macrostructures using electric field [11]–[15], a phenomenon in which a force exerted on a dielectric particle when it is subjected to an electric field (named as the dielectrophoresis [16]) is considered in this work. The strength of force strongly depends on the medium and particle electrical properties, the particle's shape and size, as well as on the frequency of the electric field. The present method based on this principle is developed for the separation of CNT fibres from each other to handle the density/porosity of CNTs in membranes. Both experiment and Dissipative particle dynamics (DPD) based numerical method have been successfully investigated for various electric fields by the alternative current (AC) of different applied voltages and frequencies.

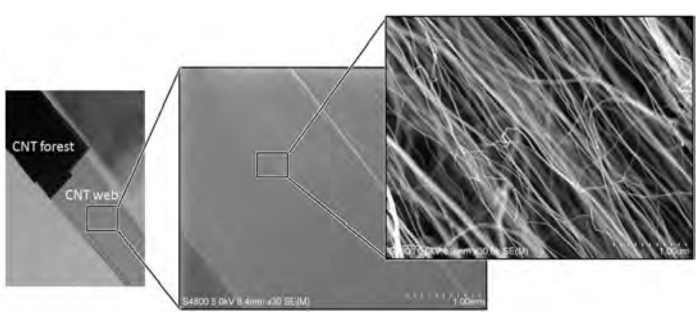

Figure 1. A structure of CNT web

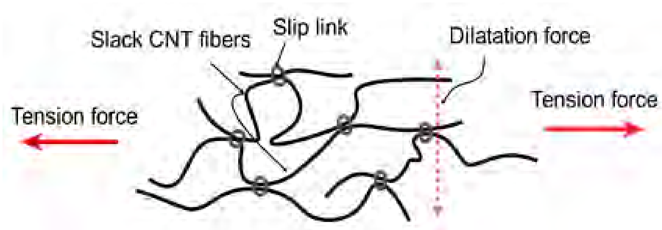

Figure 2. Dual slip-link theory based model of CNT web

2. Review on the interaction energy between CNT fibres

In macro-structures such as fibres, yarns and membranes, CNTs tend to agglomerate in the form of entangled and close-packed bundles. The interaction energy of two CNTs can be approximated by summing up the interaction between pairs of carbon atom Φ, using the Lennard Jones potential as follows [17] [18].

$$\phi(d) = 4\varepsilon\left[\left(\frac{\sigma}{d}\right)^{12} - \left(\frac{\sigma}{d}\right)^{6}\right], \tag{1}$$

where d is the distance between atomic centres; ε the depth of the potential energy well; σ the spacing where the potential energy is zero. Details of these parameters can be found in [19].

The potential energy between several two nano-structures, for example, CNT-CNT, CNT-ropes, graphene-graphene can be determined by integrating the Lennard–Jones potential over the surface of the structure using the generalized potential function [12].

$$\phi(\bar{d}) = -\frac{|\phi(d_0)|}{0.6}\left(\left(\frac{3.41}{3.13\bar{d}+0.28}\right)^{4} - 0.4\left(\frac{3.41}{3.13\bar{d}+0.28}\right)^{10}\right) \tag{2}$$

where d, d_o and ρ are the centre to centre spacing of the CNTs, the equilibrium distance (the distance between CNT centres at the unloaded state) and the distance characteristic of the specific geometries in the interaction, respectively; $|\phi(d_0)|$ the energy well depth and $\bar{d}$ is the normalized distance and given as follows

$$\bar{d} = \frac{d-\rho}{d_0-\rho} \tag{3}$$

Parameters d_o, ρ and $|\phi(d_0)|$ depend on the chiral pair of CNTs and are given in Table 1.

Table 1: Universal potential function parameters of some chiral pairs of CNTs [18]

System	Energy well depth $\lvert\Phi(d_0)\rvert$ (nJ/m)	Equilibrium spacing d_0 (nm)	Distance parameter ρ (nm)
(6,6) – (6,6) CNTs	0.1176	1.1281	0.8142
(10,10)– (10,10) CNTs	0.1525	1.6732	1.3570
(12, 12)–(12,12) CNTs	0.1674	1.9441	1.6284

In order to dilate CNT macro-structures, in the present work only the transverse extensional force will be considered and that is the basis for the dilatation of CNT bundles. From Eq. (2), the transversal force (F) per unit length required to reach a given deformation is determined as follows

$$F(\delta) = 6.119\frac{|\Phi(d_0)|}{d_0-\rho}\left[\left(\left(\frac{1}{1+0.9179\bar{\delta}}\right)^5 - \left(\frac{1}{1+0.9179\bar{\delta}}\right)^{11}\right)\right] \quad (4)$$

Where δ (δ = d - d_o) is the displacement by the transverse load, and $\bar{\delta} = \delta/(d_0 - \rho)$.

3. Dilating CNT membrane using an electrical field

In a membrane pulled out from spinnable CNT forest, bundles are oriented along the longitudinal direction in a variety of ways, some of them are bundles of parallel CNTs and others are very poorly aligned. They entangle together to create a network with an interaction energy as presented in section 2. The network entanglement impacts on the elasticity of CNT membrane through slip links (hooks) which can be movable with a constraint imposed by the surrounding CNTs. In this work, the energy and then the load to dilate CNT bundles are generated by an electrostatic field. In other words, the electrostatic potential causes the impulse force between CNT fibres to dilate bundles of CNTs.

The process is set-up as shown in Fig. 3 where a web of CNT is firstly fed through a ring. A high voltage is applied to the ring such that at a critical voltage, the repulsive force within the charged CNTs' web is against to the van der Waals between CNT bundles and the web is then spread. Stretching of CNT web depends on the voltage imposed in the ring.

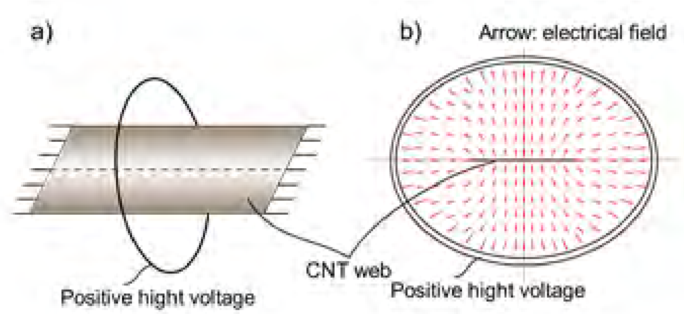

Figure 3 Dilatational separation of CNT bundles and handling CNT web density using the electrostatic field approach: a) Schematic of the separation of CNT bundles and b) A process of the dilatation of CNT bundles with electrostatic field.

As shown in Fig. 4.a, a membrane of CNT (1) of 10mm width is pulled out from a wafer of spinnable CNTs (2) grounded. A ring of 60mm diameter by steel rod of 2mm diameter is symmetrically installed surrounding the membrane (1) (Fig. 4.b). Under an electric field by different applied voltage, the CNT membrane is enlarged differently as observed in Fig. 5a & b

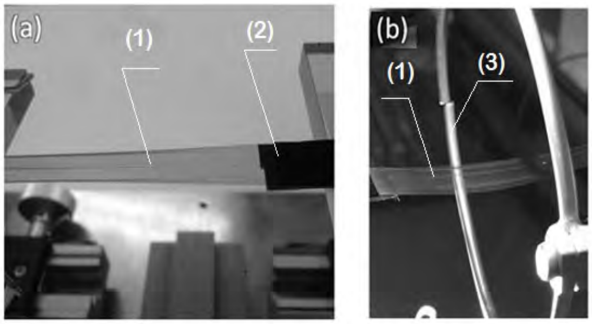

Figure 4. Experiental set-up: CNT wen inside electric field. (1) CNT membrance, (2) CNT wafer and (3) CNT ring. A range of high voltages is applied on the ring to create electric field.

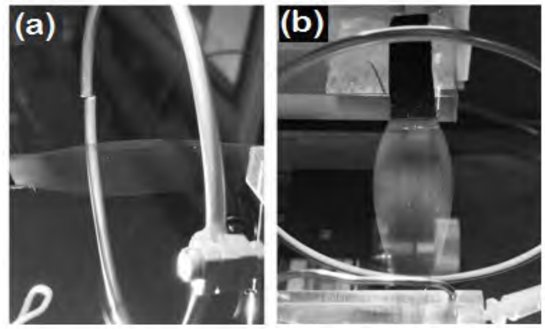

Figure 5. Experiment: Dilatational separation of CNT membranes with different electrostatic fields.

With a range of voltages from 500 V to 5000 V applied on the ring, the electric fields induce a gradual increment of the width of CNT membrane as shown in Fig. 6. The increase achieves a stable/maximum value at an applied voltage named as the critical voltage (V_{cr}) whose induced potential and force are greater than the interaction energy between CNT fibres within the membrane as presented in section 2. The interaction energy and then the force depend on the experimental parameters including the CNT membrane density, the relative dielectric coefficient and engineering parameters of ring. For example, in the condition of this experiment, the width of CNT membrane reaches a stable value (12 mm corresponding to an increase of 20%) at an applied voltage of around 4. kV (V_{cr}).

At the voltage of 4kV of the atternating current, a range of frequencies (5, 10, 30 and 100) Hz is applied to consider the response of CNT membrance. Results by Fig. 7 show that the lower frequency yields the larger width of CNT membrane at the applied voltage. For example, while the width of CNT membrance reaches the biggest increase of 20% with the frequency of 5Hz, the increase is not significant (0.3%) with the higher frequency of 100 Hz.

In summary, it can be found that the higher frequency of AC current yields the higher vibration frequency of membrane, Hence, the vibration magnitude decreases (see Fig. 8). This can be explained that since the specific frequency of the CNT film is lower that one of the used frequencies, when the frequency of impulse force is higher than the specific frequency of CNT membrane, the response of membrane is not enough fast, yielding a reduced deformation of membrane. An example of time response of magnitude variation of the CNT membrane using an applied voltage of 4kV and a frequency of 5 Hz is given in Fig. 9.

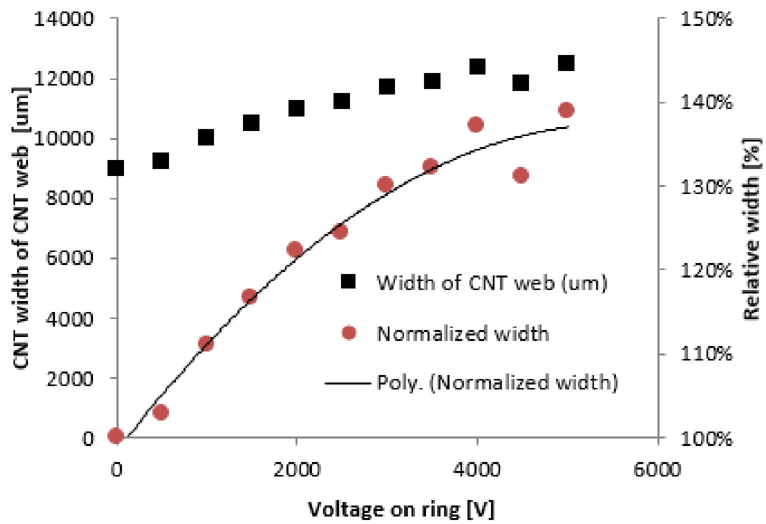

Figure 6. Experimental results: Increment of the width of CNT membrane with the electric field [0kV-5kV]: ■ Width of CNT membrane, ● Normalized width, and continuous line: the best fitting of normalised width.

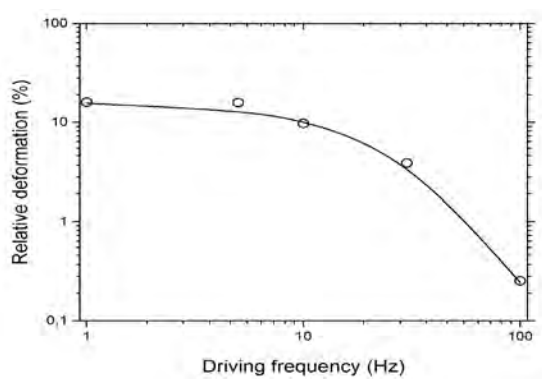

Figure 7: Variation of CNT membrane's width plotted versus the AC frequency using an applied voltage of 4kV

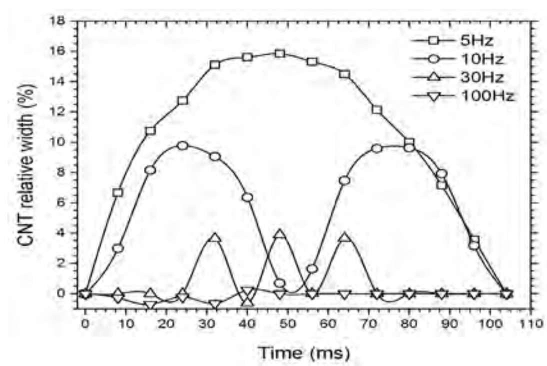

Figure 8: Frequency response with respect to time of CNT membrane width using an applied voltage of 4kV with a range of AC frequencies: 5Hz, 10Hz, 30Hz and 100Hz

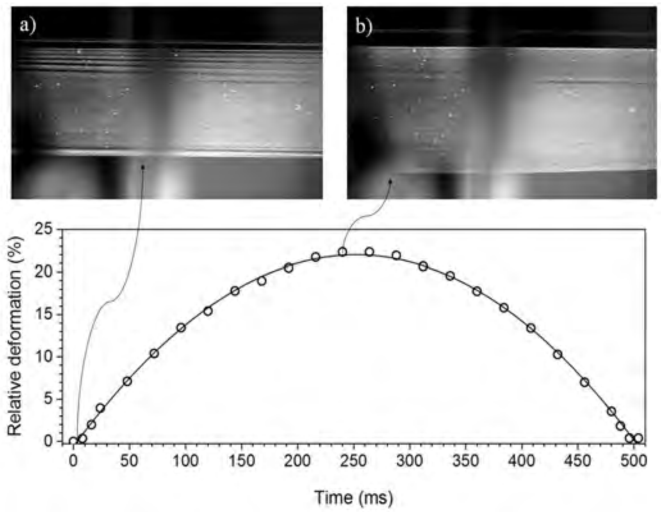

Figure 9 Dilatational separation of CNT membrane using the present method with a frequency of 5Hz and an applied voltage of 4 kV

4. Simulation of the dilatation of CNT membrane using DPD method

A numerical simulation of the present method to enlarge CNT membrane has been carried to compare with experimental results. This simulation is a multi-physical problem relating to (i) an electrical field generated by a high voltage applied on a ring to create electrostatic force on CNT membrane with residual charges; and (ii) the membrane dilatation caused by the migration of CNT fibers under the electrostatic forces. With a high voltage applied on a ring, the induced electrical potential $\phi(x, y)$is governed by the equation as follows.

$$\nabla \cdot \left(\varepsilon_r \varepsilon_0 \nabla \phi(x, y)\right) = -\rho, \tag{5}$$

where ε_r is the relative dielectric coefficient; ε_0 the vacuum dielectric coefficient (8.854E-12 F/m) and $\rho(\mathrm{x}, \mathrm{y})$ the electrical density. The electrostatic field is then determined by $\mathrm{E} = -\nabla\phi$.
Assuming that the residual charge density q on the CNT membrane, the Coulomb force given by $F_e = qE$ is introduced into the present system as body force. The dynamic response of a CNT membrane in the electrostatic field is studied using the DPD method where CNT fibers are modelled by a chain of particles whose motion is undergone by the Newton's second law. This approach satisfies conservation laws of mass and momentum and has been applied successfully for several complex-structure fluids including polymer solutions, suspensions of rigid particles, droplets, biological fluids. The CNT membrane with residual charges in CNT network is set up as shown in Fig. 3

4.1 Dissipative particle dynamics system

In the DPD system, the basic unit consists of a set of discrete momentum carriers called particles/beads that move in continuous space but in discrete time-steps. Particles are acted by three inter-particle forces: the dissipative, random and conservative forces. Hence, each particle moves with their updated velocities for a time-step after a possible collision. The time evolution of each DPD particle (*i*) governed by Newton's equation of motion for a range of time steps. DPD conserves not only the number of particles but also the total momentum of the system and satisfies Galilean invariance.

$$\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{dt}} = \mathbf{v}_i \tag{7}$$

$$m\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{dt}} = \mathbf{f}_i + \mathbf{F}_e \tag{8}$$

where $\mathbf{F}_e$ is the external force on a particle, and $\mathbf{f}_i$ ($\mathbf{f}_i = \sum_{j\neq i}(\mathbf{F}_{ij}^{C} + \mathbf{F}_{ij}^{D} + \mathbf{F}_{ij}^{R})$) the interaction force, consisting of the soft-potential conservative force ($\mathbf{F}_{ij}^{C}$), dissipative force ($\mathbf{F}_{ij}^{D}$) proportional to the velocity difference, and random force ($\mathbf{F}_{ij}^{R}$) modelled by white noise. The random and the dissipative forces are center -to-center and pairwise additive. The interaction forces are given in Table 2.

Table 2. List of interaction forces and weight functions. $\boldsymbol{r}_i$ and $\boldsymbol{v}_i$: the position and velocity of DPD particle *i;* $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$, $r_{ij} = |\boldsymbol{r}_{ij}|$, $\boldsymbol{v}_{ij} = \boldsymbol{v}_i - \boldsymbol{v}_j$; r_c: the cut off radius; a_{ij}: maximum repulsion between particles i and j; ξ_{ij}: the Gaussian random variable; γ and σ: the amplitude of dissipative and random forces, respectively

$\mathbf{F}_{ij}$	Forms	Weight functions
$\mathbf{F}_{ij}^{C}$	$a_{ij}w^{c}\hat{\boldsymbol{r}}_{ij}$	$w^{C}(r_{ij}) = 1 - r_{ij}/r_c$
$\mathbf{F}_{ij}^{D}$	$-\gamma w^{D}(\hat{\boldsymbol{r}}_{ij}\cdot\boldsymbol{v}_{ij})\hat{\boldsymbol{r}}_{ij}$	$w^{D}(r_{ij}) = (1 - r_{ij}/r_c)^{s}$
$\mathbf{F}_{\boldsymbol{ij}}^{\boldsymbol{R}}$	$\sigma w^{R}\xi_{ij}\hat{\boldsymbol{r}}_{ij}$	$w^{R}(r_{ij}) = \sqrt{w^{D}(r_{ij})}$

4.2. *DPD modelling of CNT chains*

By connecting DPD particles and spring forces, CNTs can be modelled by the DPD method. The spring model for CNT chains is constructed by linking a series of DPD particles together with spring forces acting between adjacent particles of a CNT as shown in Fig. 10. The force on particle *i* due to particle *j* is given by

$$\mathbf{F}_{ij}^{s} = -\frac{\mathbf{H}\mathbf{r}_{ij}}{1-\left(\mathbf{r}_{ij}/\mathbf{r}_{m}\right)^{2}} \quad , \tag{9}$$

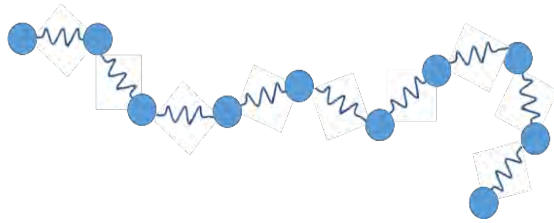

Figure 10. Model of a CNT fiber consisting of several DPD particles connected by springs where H is the spring constant and r_m the maximum length.

van der Waals interactions between the CNTs are represented by simple modifications of the DPD inter-particle forces. The modified version of DPD is developed by introducing a long-range attractive component into the conservative forces. A new conservative particle-particle interaction combining short-range repulsive and long-range attractive interactions to simulate van der Waals interactions. New conservative force between CNT chains $\mathbf{F}_{ij}^{c}$ is calculated by taking derivative with respect to $\boldsymbol{r}$ of a potential like Lennard-Jones potential with attractive and repulsive terms [20].

$$\mathbf{F}_{ij}^{c} = -a_{ij}\left(\mathrm{A}w_{r}^{c}(r, r_{cr}) - \mathrm{B}w_{a}^{c}(r, r_{ca})\right)\hat{\boldsymbol{r}}_{ij} \tag{10}$$

where A and B are coefficient of $\boldsymbol{w}_{\boldsymbol{r}}^{\boldsymbol{c}}(\boldsymbol{r}, \boldsymbol{r}_{\boldsymbol{cr}})$ and $\boldsymbol{w}_{\boldsymbol{a}}^{\boldsymbol{c}}(\boldsymbol{r}, \boldsymbol{r}_{\boldsymbol{ca}})$, respectively; $\boldsymbol{r}_{\boldsymbol{cr}}$ the cut-off radius of repulsive component, $\boldsymbol{r}_{\boldsymbol{ca}}$ radius of attractive component and

$$\mathbf{w}_{\mathbf{r}}^{\mathbf{c}}(\mathbf{r}, \mathbf{r}_{\mathbf{cr}}) = \begin{cases} -12\frac{r}{r_{\mathrm{cr}}^{2}} + \frac{18r^{2}}{r_{\mathrm{cr}}^{3}}, & r < \frac{r_{cr}}{2} \\ -\frac{3}{2r_{cr}}\left(2 - 2\frac{r}{r_{\mathrm{cr}}}\right)^{2}, & \frac{r_{\mathrm{cr}}}{2} < r < r_{\mathrm{cr}} \\ 0, & r > r_{\mathrm{cr}} \end{cases} \qquad \mathbf{w}_{\mathbf{r}}^{\mathbf{c}}(r, r_{ca}) = \begin{cases} -12\frac{r}{r_{ca}^{2}} + \frac{18r^{2}}{r_{ca}^{3}}, & r < \frac{r_{\mathrm{ca}}}{2} \\ -\frac{3}{2r_{ca}}\left(2 - 2\frac{r}{r_{\mathrm{ca}}}\right)^{2}, & \frac{r_{\mathrm{ca}}}{2} < r < r_{\mathrm{ca}} \\ 0, & r > r_{\mathrm{ca}} \end{cases}$$

It can be seen by Fig. 11 that the conservative force among different CNT's particles is repulsive (the positive part) when their separation distance is less than the value of radius $\boldsymbol{r}$ (e.g. 0.5952 with $\mathbf{A} = \mathbf{2}, \mathbf{B} = \mathbf{1}, \boldsymbol{r}_{\mathbf{cr}} = \mathbf{0.8}, \boldsymbol{r}_{\mathbf{ca}} = \mathbf{1}$) and when their separation distance falls in the range between 0.5952 and 1, this force describes a long range attraction (the negative part).

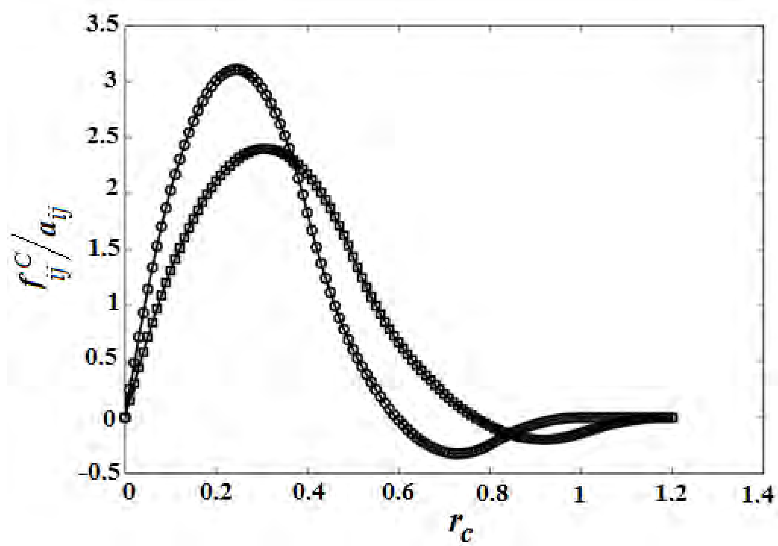

Figure 11: Conservative force with short range repulsion and long range attraction (**–o-**: r_a = 1.0) and (–□– : r_a = 1.2)

4.3. *Computational parameters of the problem, results and discussions*

A non-dimensional 3D domain of 40 x 9 x 1 (length x width x thickness: unit^3) claimed at two ends as shown in Fig. 12 (also see Fig. 3a). The simulation is performed in the constant number of DPD-CNT beads and constant temperature ensemble. One CNT fibre is considered as a rigid body and modelled as 10 DPD particles linked together by 9 spring chains (Fig. 11). It is worth noting that the balance between dissipative and random forces must satisfy the fluctuation-dissipation theorem [22],[23]. This means that the dissipative parameter (γ) should be proportional to the noise parameter (σ) $\sigma = \sqrt{2\gamma k_B T}$. It is recommended that σ should be chosen appropriately for maintaining stability of the system, as well as quickly reaching the temperature equilibrium [23]. Thus, the DPD parameters are determined for the present work as follows: $m_i = 1,\ a_{ij} = 18.75,\ \ \gamma = \sigma^2 = 4.5$, $r_{cr} = 0.8, r_{ca} = 1.3$. The density of CNT membrane is 7 DPD particles per a unit cube. A total of 500 chains is generated as depicted in Fig 3.a and Fig. 12a. For the conservative force of DPD, the strengths of repulsive and attractive parts (See Fig. 9) are the value of A = {1} and B = {0.1}, respectively.

Periodic boundary conditions are applied in y-direction meanwhile in x- and z-directions, solid walls are represented by three layers of frozen particles (see Fig. 12a). In the following simulations, the Verlet integration algorithm is employed to solve Eqs. (7) & (8). The simulation is run with 240,000 time steps and a unique time step of 10^{-2} is chosen for all simulations for a range of voltages from

500V to 5000V applied on the ring. Body force caused by the electrical field from the applied voltage on the ring.

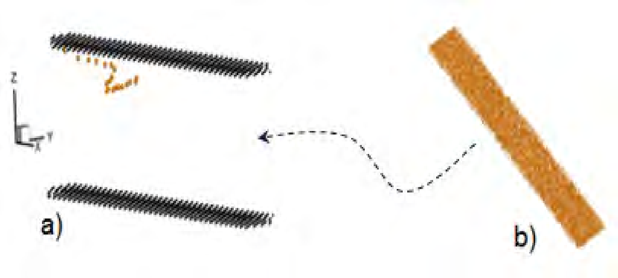

Figure 12. Simulation domain: (a) 3D view of a spring model of a single CNT moving between two walls and (b) A CNT membrane represented by 500 DPD chains

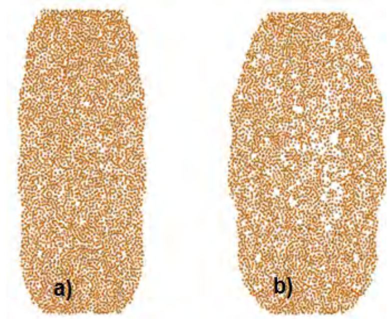

Figure 13. Numerical visualization of width of CNT membrane increased (120% (a) and 140% (b)) with respect to the electric field.

Figure 14 shows the increment of membrane width with respect to voltages applied on ring (triangles in the figure) and the simulated results are in good agreement with those by experiment expressed by red circles. For example, an increase of 120% and 140% for the normalised width of the CNT membrane at the centre of CNT membrane corresponding to 2kV and 5kV respectively as shown in Fig 13. More details and investigations on the simulation using DPD method for processing CNT macrostructures will be presented in our future modelling and simulation work.

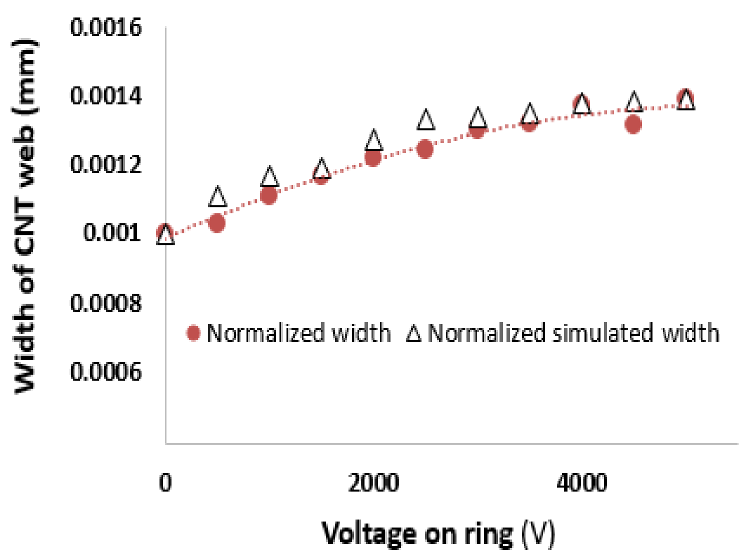

Figure 14. Comparison of the CNT membrane width plotted versus the applied voltage on ring by experiment and numerical method

5. Several potential applications

The experimental and numerical results are the basis to develop processes and techniques for producing CNT membranes and yarns whose structure can be well processed. Such CNT membranes and yarns are efficiently used as sensors [9], [10], [24]–[26] . The following works have been initially carried out and attained some promising results.

5.1 Multi-step CNT spinning process

Although the recent modified dry spinning process leads to a significant improvement of the properties of a CNT yarn [2], there exists some limits in enhancing the CNTs' alignment in a web because of the fragility of CNT webs while enlarging CNT membranes using mechanical treatment methods. The dilation of membrane using the dielectrophoresis technique allows easily developing a multi-step CNT spinning process (Fig. 15) which further enhances mechanical properties of CNT macrostructures.

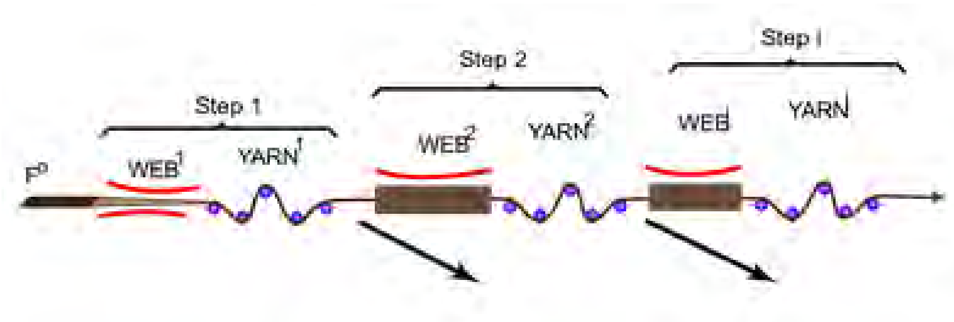

Figure 15 Schematic of the process of multi-step spinning model combined with the dielectrophoresis technique: a) step1: initial CNT web; b) step 2: CNT sliver at the first phase and c) CNT sliver at the second phase etc.

With the introduction of the dilatation into the yarn spinning process, the experimental observation found that the alignment of CNTs in a web is gradually improved through the spinning steps and the damage of CNT bundles is significantly reduced [3].

5.2 Manufacturing functional polymer/CNT membranes

A combination between the CNT membrane process using the electric field and polymer nano-fibre electro-spinning technique yields producing functional CNT/polymer macro-structures satisfying various engineering requirements such as absorptive materials and bio-filters where the density of CNTs as well as the porosity of the media can be handled.

Figs. 16 presents the SEM images of several sandwiches of the CNT and polymer fibers by electrospinning technique and CNT membranes treated by the electric field. The multi-layer membranes produced by the present scheme can satisfy requirements on the mechanical and physical properties including the porosity, tenacity and absorbability.

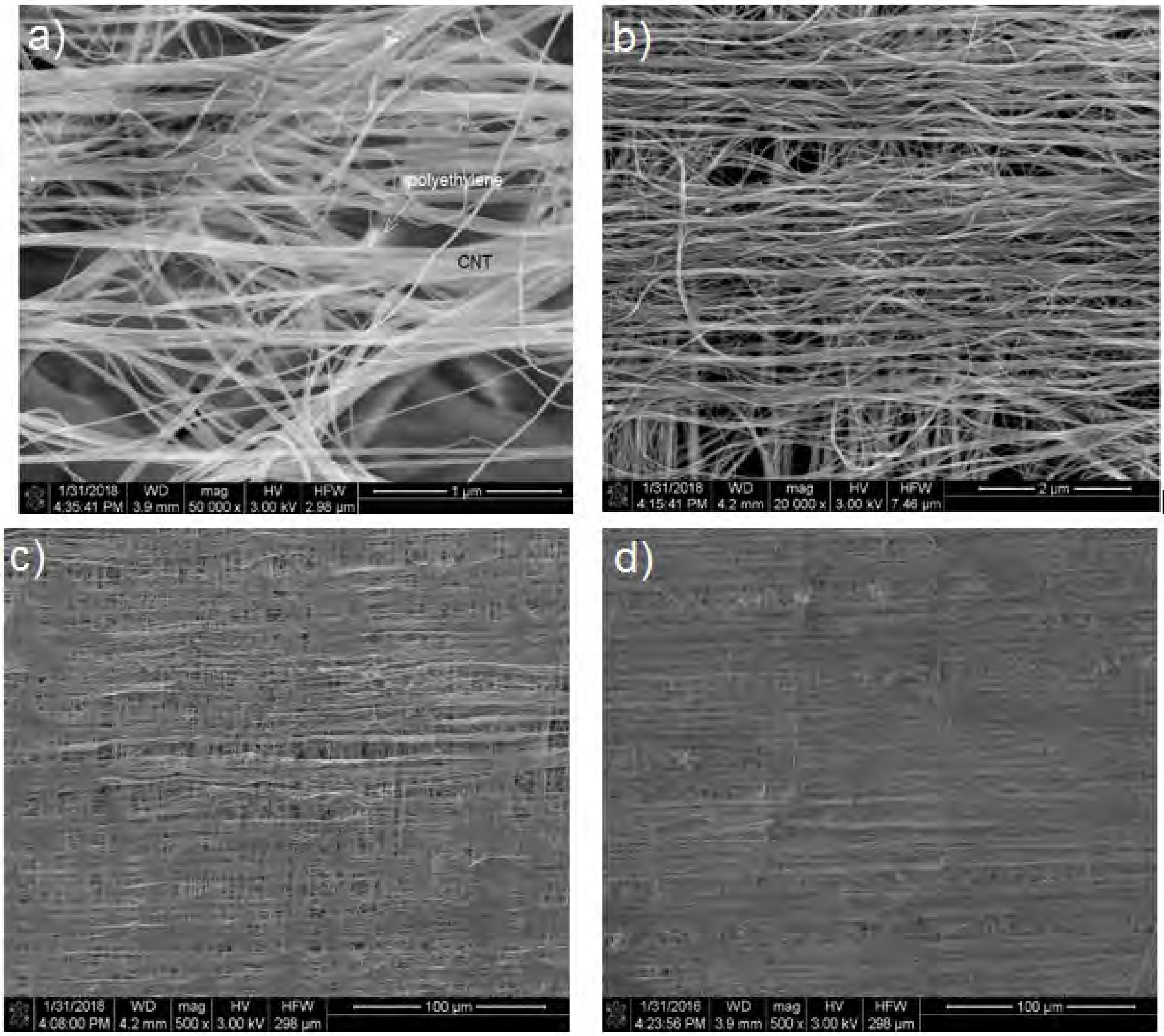

Figure 16 SEM images of functional multi-layer macrostructures: poly-urethane nano-fibers spayed on CNT membrane of two directions with different magnifications.

6. Conclusion

This paper reports an approach to process CNT membranes using the present dielectrophoresis method where CNT fibres are separated from each other in webs as well as CNTs based macrostructures. This helps partially eliminate the agglomeration of CNTs and other nano-particles into in several different processing. The present method based on the slip-link entanglement model and the electric field technique to separate CNTs from bundles. The work then devises a new process to handle the density/porosity which affects physical and mechanical properties of CNT macrostructures. A particle base numerical method has been used to simulate the dilation process whose results are in very in good agreement with those by the experiment. Finally, several potential applications of the present technique have also been presented.

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