Processing the CNTs' interaction in web using an electro-static field based process

Canh-Dung Tran[1*], Thanh Tran-Cong[1], Le-Cao K[1] and Ho-Minh D[1]

[1]Computational Engineering and Science Research Centre (CESRC), Faculty of Engineering and Surveying, University of Southern Queensland, Toowoomba, QLD 4350, Australia

*Corresponding author: Email canh-dung.tran@usq.edu.au

Abstract: CNTs are not individualised in the web, instead they tend to be agglomerated into bundles because their substantial length-to-diameter ratio promotes quite strong van der Waals interaction [1]. CNTs usually form into bundles containing up to hundreds or thousands of parallel CNTs and these have been described as nanoropes [2]. The present method aims to analyse the CNT's interaction in macro-structures as well as how to separate nanotubes from bundles and then devise a new process to handle the density of macro-structures based on the electrical/magnetic and mechanical properties of CNTs.

Potential energy function for the interaction between CNTs: The interaction energy of two CNTs can be approximated by summing up the interaction between pairs of carbon atom, using the Lennard Jones potential [3-6].

Recently Girifalco et al. [3] have developed a continuum approach to calculate the potential between two nano-structures (for example, CNT-CNT) by integrating the Lennard–Jones potential over the surface of the structure. In order to separate the CNTs, the transverse extensional force will be the basic for the dilatation of CNT bundles. The energy and force per unit length required to reach a given deformation are determined, respectively as follows

$$U(\delta) = \Phi(d) - \Phi(d_0) = |\Phi(d_0)|\left[1 - \frac{1}{0.6}\left(\left(\frac{1}{1+0.9179\bar{\delta}}\right)^{4} - 0.4\left(\frac{1}{1+0.9179\bar{\delta}}\right)^{10}\right)\right] \quad (1)$$

$$F(\delta) = 6.119\,\frac{|\Phi(d_0)|}{d_0 - \rho}\left[\left(\left(\frac{1}{1+0.9179\bar{\delta}}\right)^{5} - \left(\frac{1}{1+0.9179\bar{\delta}}\right)^{11}\right)\right] \quad (2)$$

where $\bar{\delta} = \delta/(d_0 - \rho)$, d_o, d and ρ are the distance between centres of CNTs before and after transverse load and length characteristic of the specific in the interaction, respectively; δ (δ = d - d_o) is the displacement and $|\phi(d_0)|$ is the energy well depth. d_o, ρ and $|\phi(d_0)|$ depend on the chiral pair of CNTs and are given in [3].

Processing CNTs' interaction in web using electrostatic/magnetic field approach: In the web formed from the forest, the bundles are oriented along the draft direction. It is desirable to have an aligned network of bundles of CNTs in the web structure as well as control the coagulation of CNTs. The present electrostatic field approach allows for controlling the CNTs' density in macrostructures.

Dilatational separation of CNT bundles: The dilatation of CNT bundles will be carried out by the transverse extensional force. Considering a hexagonal bundle of a finite number (N) of CNTs (Fig. 1), the energy density (per unit volume) needed to separate the bundle into individual CNTs is given by [3]

$$E = \frac{4\Phi(d_o)}{\sqrt{3}d_0^2}\,\frac{\sum_{i=1}^{N}(3i-1)}{\sum_{i=1}^{N}(2i-1)} \quad (3)$$

where i is the characteristic coefficient of the hexagonal array of CNTs, the number of CNT centre-to-centre lengths that make-up the length of a side of the hexagon encompassing all unit cells in the array.

Separating CNT web using an electrostatic field: In the present work, the energy for controlling CNTs' interaction in bundles (and then a web) is set up using an electrostatic/magnetic field. The electrostatic potential causes the impulse force between parallel CNTs and separates the bundles into CNTs.

The process is set-up as shown in Fig.2 where a web of CNT is first fed through a ring. A high voltage is applied to the ring such that at a critical voltage, typically more than 4 kV, the repulsive force within the charged CNTs' web is against to the van der Waals between CNTs and the web is then spread. Stretching of CNT web depends on the electrostatic forces caused by the voltage imposed in the ring. Fig. 3 showed the electric field using the electrostatic approach set up as described in Fig. 2. Since the electrostatic charges are distributed along the CNT web, the control of the electrostatic field allows to handle the density and alignment of CNTs in the webs (Fig. 4). The achieved results are the basis to develop new processes for producing CNT membranes and yarns whose structure (CNTs' density) is controllable. In fact, a novel multi step spinning process using this technique and based on the modified spinning process [2, 7] for further improvement of CNT macro-structures has been successfully developed and will be presented at the conference.

Acknowledgements

This research was supported by a collaborative research grant from CSIRO Future Manufacturing Flagship.

References

[1] L.A. Girifalco, M. Hodak and R.S. Lee, Phys. Rev. B, 62(19), pp. 13104–10, 2000.

[2] C.D. Tran, W. Humphries, S.M. Smith, C. Huynh and S. Lucas Carbon, 47, pp. 2662-2670, 2000.

[3] L.A. Girifalco, M. Hodak and R.S. Lee Phys. Rev. B, 62(19), pp. 13104–10, 2000.

[4] J. Tersoff and R.S. Ruoff. Phys. Rev. Lett. 73, pp. 676–9, 1994.

[5] L.A. Girifalco, J. Phys. Chem., 96(2), 858–61, 1992.

[6] L.A. Girifalco, R.A. Lad, J. Chem. Phys. 25(4), 693–7, 1956.

[7] C.D. Tran, S. Lucas, D.G. Phillips, R.H. Baughman and T. Tran-Cong, *Nanotechnology,* **22,** 1453021-9, 2011

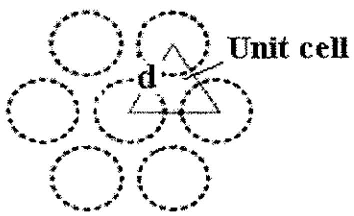

Fig.1. Schematic of the cross-section of a hexagonal array of CNTs.

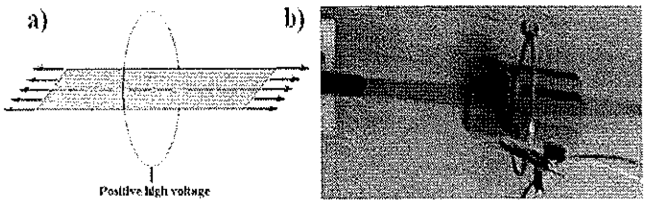

Fig.2 Dilatational separation of CNT bundles and control of CNT web density using the electrostatic field approach: a) Schematic of the dilatational separation of CNT bundles and b) A real process of the dilatational separation of CNT bundles.

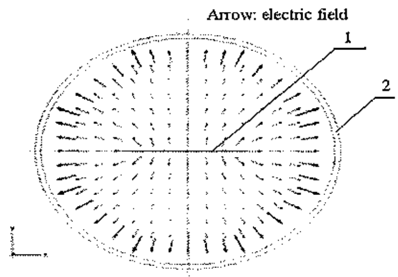

Fig.3. Electric field from electrostatic approach: CNT web (1), ring of high voltage (2). Arrows depict the electric field

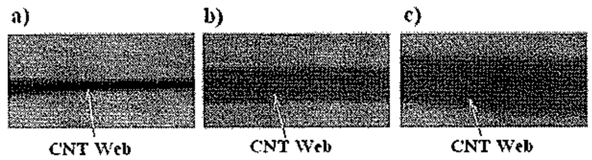

Fig.4 Density of CNT web with different magnitudes of electric field carried out at USQ: a) Without electric field; b) Electric field of 4 kV voltage and c) Electric field of 7 kV voltage.