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Multiscale Structural Model of Super Carbon Nanotubes

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Abstract

Extraordinary mechanical properties in biological composites come from their hierarchical structures and are well seen in bones, teeth, shells etc. Nature inspired knowledge could certainly help in the design of new nanostructured materials. The current study illustrates a multi-scale nanotube model for the purpose of the structure of very large groups of carbon nanotubes (CNTs). Two different types of circular beam finite elements are used to shape bond stretching energy or to account for the potential connected to bond angle variation. Multiscale approach considers CNTs at a mesoscopic level through chains of straight cylindrical segments, where mesoscopic force field describes the interactions among the segment. Property dependence at the nanoscale results from the surface and bulk energies competition.

Keywords: Hierarchy; Super Carbon Nanotube; Numerical Model

1 Introduction

For a material to have superior mechanical properties the limits of improving one property by sacrificing another should be overcome. Hierarchical structures of exceptional properties are widespread in biosystems such as bones, teeth, shells, collagen tissues etc. The knowledge on hierarchical biomaterials could obviously help design new nanostructured technical materials and products. Thus, scientists are suggesting materials property control at multiscale levels. Mathematical models involved in hierarchical materials design reported consider: self-similar and multiple reinforced composites, bio-inspired structures, ceramic based nanocomposites and fibre reinforced composites. The methods used are based on global-local finite element, domain decomposition and superposition techniques [1-3].

The fourth allotrope of condensed carbon is carbon nanotube. Carbon nanotubes are rolled-up cylinders of graphene sheets with tubule diameters sometimes small to have 1D periodicity. Plenty of attention is paid to carbon nanotubes (CNTs) because of their special structural and transport features, including excellent tensile strength, high modulus, good electrical and thermal conductivity and low density [4-6]. Significant mechanical and physical properties of individual

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carbon nanotubes encourage researchers to develop continuous high performance fibres and ropes based on carbon nonotubes. Some studies reported on the molecular mechanics modelling of the pull-out force between adjacent CNTs in double wall carbon nanotubes [7], others focused on super-nanotubes super-graphene and super-square systems continuum modelling, with the use of equivalent beam concept [8]. Nanostructures with an optimal distribution of nanoelements (nanoclay, carbon nanotubes, nanoparticles and nanofibres) enable a great increase in properties and functionality [9]. Some microstructure recipes such as multilayer configuration, hierarchical tree structures, bundle and yarns can be considered as elements of the bio-inspired design of industrial materials.

A number of carbon nanotubes have been assembled by hierarchical super carbon nanotubes (SCNT). Lowest order (SCNT) is the building block of the second one, and the latter for the next one and so on, Fig. 1. Thus a kind of hierarchical structure can be obtained with exceptional properties, not existing in original structures previously [1, 10].

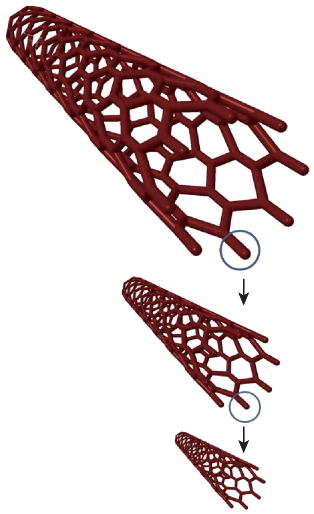


Fig. 1: The hierarchical CNT super structure

Macro-scale super carbon tubes were investigated because of self-similarity breakage [11]. In this study an example of the super CNTs numerical nanostructure modelling is carried.

2 Numerical Model-carbon Nanotubes Super Structures

Materials are modelled using phenomenological/continuum models or force constant, bond angle bending force constant and torsion resistance respectively and quantum/molecular mechanics models. However, the material length and time scales for the molecular mechanics model simulations are still limited by the available computational power, and such methods are prohibitive in the analysis of nanoscale devices. It is therefore important to extend the multiscale mechanics concepts as an efficient tool to analyse the mechanical response of nanoscale structures. For the analysis of complex nanostructures geometries and boundary conditions encountered in nanotechnology applications, a versatile numerical model such as the coarse-grain method, quasi-continuum method, concurrent and hierarchical multiscale method was developed.

2.1 Molecular Structural Mechanics (MSM) Method

The general expression for total potential energy without electrostatic interaction is the total amount of energies because of valence or bonded interactions and non-bonded interactions, respectively

$$U = \sum U_r + \sum U_\vartheta + \sum U_\phi + \sum U_\omega + \sum U_{vdw} \tag{1}$$

where U_r is for bond stretch interaction, U_ϑ for bond angle bending, U_ϕ for dihedral angle torsion, U_ω for out-of-plane torsion, and U_{vdw} for non-bonded van der Waals interaction. Every carbon atom acts as the bond of related load bearing beam members, Fig. 2.

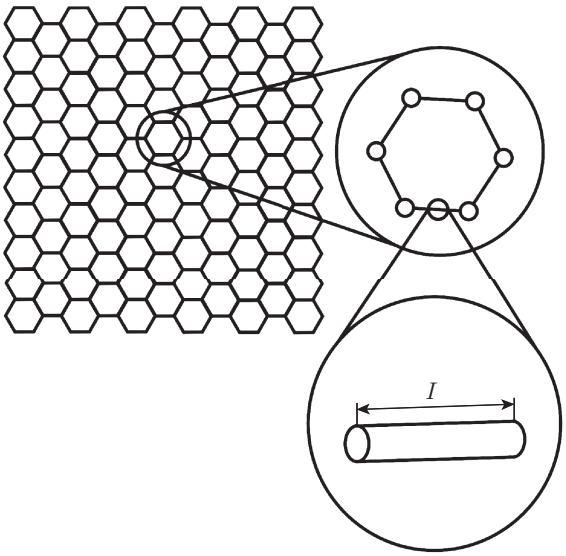


Fig. 2: The molecular-structural mechanics analogy

In terms of the theory of classical structural mechanics strain energy of a beam/truss member is

$$U = \frac{1}{2}\int_0^l \frac{N^2}{EA}ds + \frac{1}{2}\int_0^l \frac{M_B}{EI}ds + \frac{1}{2}\int_0^l \frac{M_T^2}{GJ}ds \tag{2}$$

where N, M_B and M_T mean axial force, bending or torsion moments applied on the beam. The connection between structural and molecular mechanics using equivalence of energies creates the following relationships.

$$\frac{EA}{l} = k_r \quad \frac{EI}{l} = k_\vartheta \quad \frac{GJ}{l} = k_\tau \tag{3}$$

where A is cross sectional area, E modulus of elasticity, I and J axial and polar moments of inertia of the cross-section, and l is element length. The atomic finite element procedure method for CNT as space frame structures [12], results with matrix equation

$$[K]\{\delta\} = \{F\} \tag{4}$$

where $[K]$, $\{\delta\}$ and $\{F\}$ are element stiffness matrix, displacement vector and force vector, respectively.

2.2 Mesoscopic Model of CNTs Structures

This study deals with the multi-scale development model for nanotube representation in order to make possible the simulation of structural organization of very large bundles of CNTs. The continuum theory determining the equation for bundle formation and equilibrium was described using energy balance between bending strain energy, local deformation contact energy and adhesion energy. At the nanoscale, weak van der Waals interactions control the structure and the mechanical properties of CNT based structures. High axial strength of individual nanotubes goes lost when nanotubes form bundles as weak forces allowing slippage of nanotubes within a bundle [13]. An alternative multiscale approach, as applied here, represents CNTs at a mesoscopic level through chains of straight cylindrical segments, Fig. 3 [14]. The purpose of mesoscopic model is to develop a computationally efficient approach in order to show non-bonding interactions among CNTs. The model presented here describes only the basic elements necessary for performing mesoscopic simulations between interacting CNTs. The nodes divide CNTs into segments, where each segment is defined as a straight cylinder of a CNT between two neighbouring nodes. In the system of N CNTs, n_i nodes describe each nanotube $i(i = 1, \ldots, N)$, Fig. 3. Nanotube i can is characteristic for a set of position vectors $r_{i,j}$ of its nodes, $q_i = (r_{i,1}, \ldots, r_{i,Ni})$, so that the pair $(r_{i,j}, r_{i,j+1})$ defines the position and orientation of segment$j$ of the nanotube i.

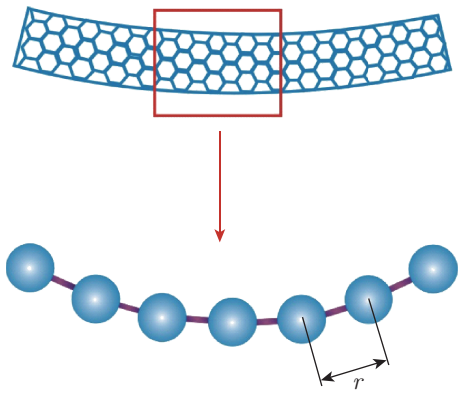


Fig. 3: CNT as coarse-grain system

The behaviour of the system can be described by using equations of motion of classical mechanics in the Lagrangian form [14]

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0 \tag{5}$$

where $q = \{q_1, q_2, \ldots, q_N\}$ is vector generalized coordinates.

$L = E - U$ is the Lagrangian of the system. E and U are kinetic and potential energies of the system. The total potential energy of the system is expressed by

$$U(q) = U_s(q) + U_B(q) + U_{INT}(q) \tag{6}$$

where Us is potential energy of nanotube stretching, U_B is bending and inter-tube interaction U_{INT}. The calculation of the CNT-CNT interaction potential U_{INT} is given by two successive steps.

CNT-CNT interaction potential on the right side of Eq. (6) can be decreased to the interactions between the pairs of segments:

$$U_{INT}(q_i, q_j) = \sum_{k}^{N_i-1} \sum_{l}^{N_j-1} \Im\left(r_{i,k}, r_{i,k+1}, r_{j,l}, r_{j,l+1}\right) \tag{7}$$

where $\Im$ is the potential energy of interaction between two similar segments.

An efficient method for the calculation of $\Im$ is based on continuum approach, where the total amount of interatomic integrations is replaced by the surface integration of the interacting segments. Now, the segment-segment potential can be determined by integrating modified Lennard-Jones potential $\Psi(\ldots)$ over the surfaces of interacting segments:

$$\Im(h, \alpha, \xi_1, \xi_2, \eta_1, \eta_2) = \rho \cdot R^2 \iiint\!\!\!\iint (h, \alpha, \xi, \phi_1, \phi_2) d\phi_1 d\phi_2 d\eta d\xi \tag{8}$$

Finally, six geometric parameters h, α, ξ_1, ξ_2, η_1 and η_2 establish the relative position of two segments in relation to each other, Fig. 4.

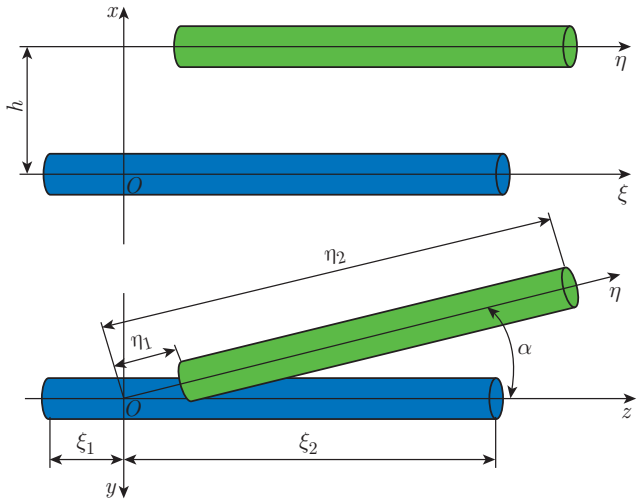


Fig. 4: Illustration of interaction of two CNTs

3 Results and Discussion

The space-frame of the carbon nanotubes (CNT) model is designed by two different types of circular beam finite elements. A different Cants type with representative volume element has been selected for the present work, including zigzag and armchair. The effective axial Young modulus is determined from following relation

$$\langle E \rangle = \frac{\langle \sigma \rangle}{\langle \varepsilon \rangle} \quad \text{with} \quad \langle \varepsilon \rangle = \frac{\Delta l}{l} \tag{9}$$

where: Δl is CNT incremental displacement, $\langle \sigma \rangle$ is effective axial stress,

$$\langle \sigma \rangle = \frac{1}{V} \int_V [D][B]\{u\} dV \tag{10}$$

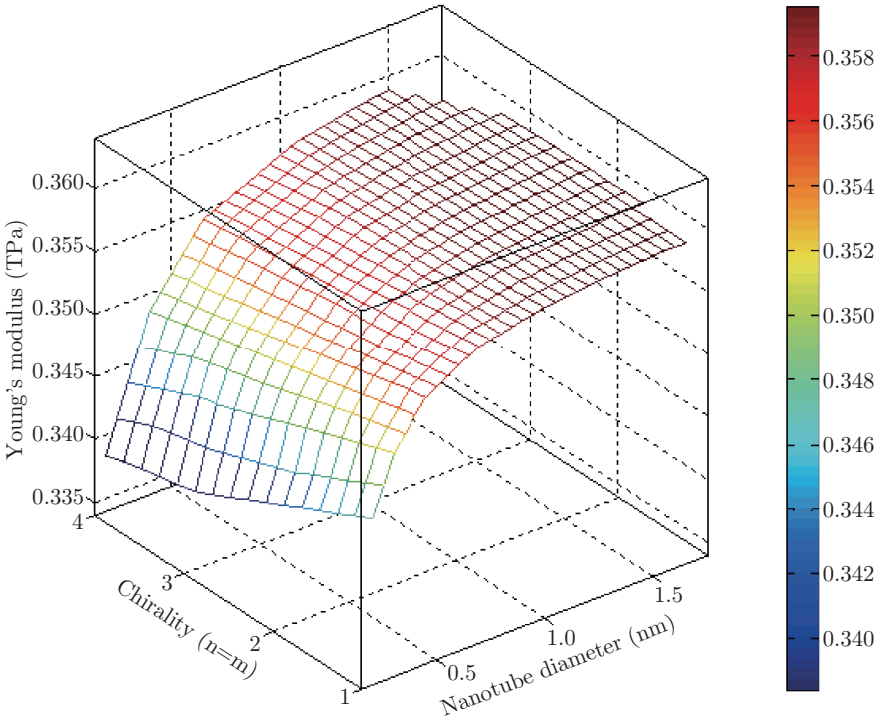


Fig. 5: The effective Young modulus dependence on chiralities and CNT radii

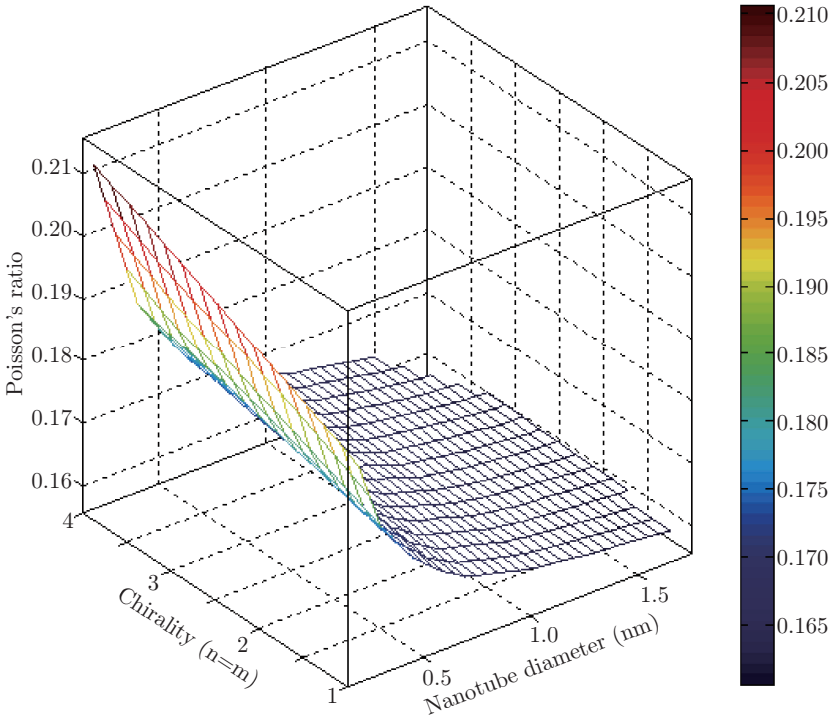


Fig. 6: The effective Poisson ratio dependence on chiralities and CNT radii

determined by finite element procedure for CNT representative volume element V (example in [15]). The matrices $[D]$ and $[B]$ are elasticity matrix and gradient displacement matrix respectively. The effective Poisson ratio $\langle\nu\rangle$ is determined on the some way. The influence of chiralities and CNT radii on effective Young modulus and Poisson ratio are presented in Fig. 5

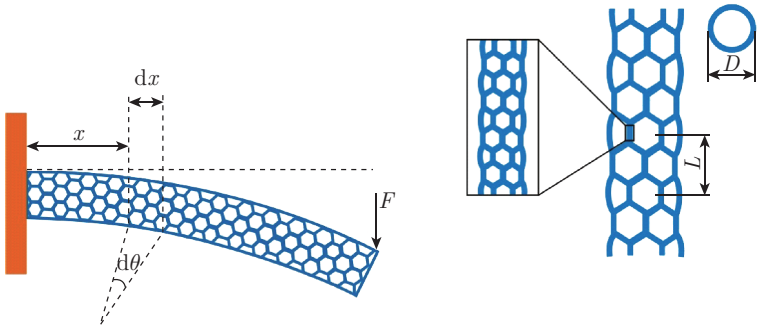


Fig. 7: Super carbon nanotube as cantilever under bending

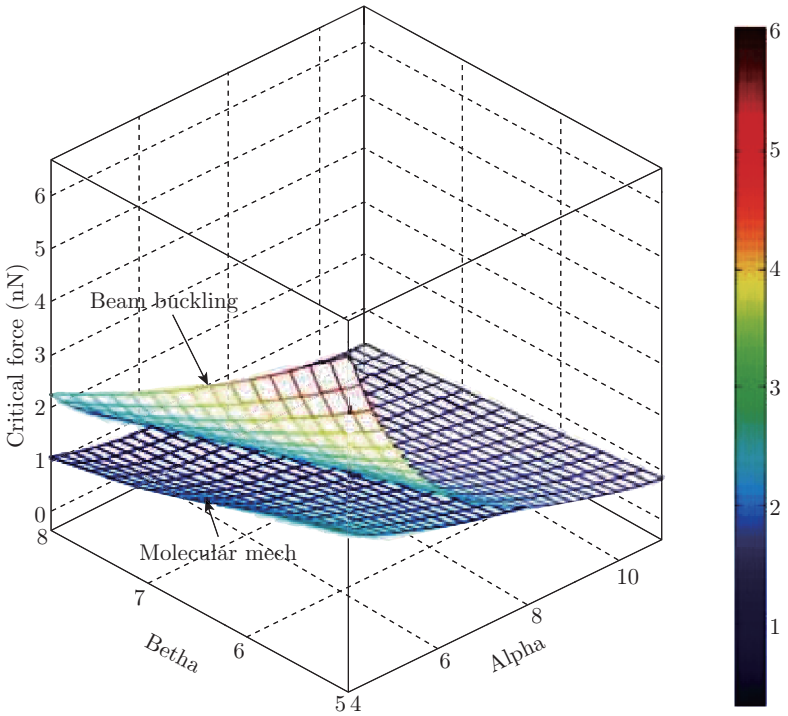


Fig. 8: Critical bending forces dependence on slenderness parameters α and β

and Fig. 6. Molecular simulations have been performed by many researchers to confirm the strong size-dependency on nanostructures properties.

The MSM method can be generalized for structural analysis of super CNT structures. In order to show accuracy and wide application of MSM method, the buckling of super CNT is also analysed. The cantilever [6, 0]@(6, 0) super carbon nanotubes defined by two structural parameters, Fig. 7.

$$\begin{aligned} \alpha &= L/D \\ \beta &= l/d \end{aligned} \tag{11}$$

where L and D is the length and diameter of super CNT, l and d, are length and diameter of CNT as a building element, respectively. The critical buckling load is determined by the classical Euler beam formula [16] and MSM method, Fig. 8. It is evident that super carbon nanotube need to be modelled as shell structure.

4 Conclusion

The design of multiscale nanostructure, hierarchy and construction of material properties by controlling the structure at various levels have a potential to improve the quality of different mechanical properties. Effective elastic properties of carbon nanotubes are determined by atomic finite element method. The basic cause of the size properties at the nanoscale is the competition between surface and bulk energy.

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