Computers and Structures 195 (2018) 126–144

Contents lists available at ScienceDirect

Computers and Structures

journal homepage: www.elsevier.com/locate/compstruc

A computationally efficient multiscale finite element formulation for dynamic and postbuckling analyses of carbon nanotubes

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ARTICLE INFO

Article history:
Received 27 October 2016
Accepted 10 October 2017
Available online 19 October 2017

Keywords:
Carbon nanotube
Finite element
Membrane locking
Molecular mechanics
Nonlinear response
Multiscale modelling

ABSTRACT

The efficient multiscale membrane locking free shell elements are developed to study the dynamic and postbuckling characteristics of carbon nanotubes incorporating material and geometric nonlinearities. The constitutive relation at continuum level is derived through the Cauchy–Born rule incorporating the effect of curvature tensor on bond lengths and using the Tersoff–Brenner atomic interaction potential per unit area of a unit cell. The membrane locking is eliminated by using the smoothed shape functions derived through the least square strain smoothing technique for the interpolation of the transverse displacement in the circumferential strain. The performance of the four/eight noded inconsistent/consistent Kirchhoff rectangular and improved discrete Kirchhoff quadrilateral (IDKQ) shell elements is investigated. It is found that the four noded elements with smoothed interpolation of transverse displacement in the circumferential strain yield accurate results and are computationally efficient. The multiscale modelling results are found to be in close agreement with the molecular mechanics simulations. The significant effect of material nonlinearity on the nonlinear dynamic and postbuckling responses is predicted.

1. Introduction

The exceptional properties of carbon nanotubes (CNTs) accelerated their engineering applications in sensing/actuation, load bearing members, oscillators, manufacturing and medicine etc. For the design of such devices, their dynamic characteristics are important. Limited experimental studies have been carried out on static and dynamic behaviour of single walled/ multi walled carbon nanotubes (SWCNTs/MWCNTs) [1–4]. Further, the mathematical modelling and analysis of CNTs is explored as an efficient tool to understand their structural behaviour using continuum modelling, molecular mechanics/dynamics simulations, stress and strain gradient nonlocal theories, multiscale modelling.

For the long CNTs with length to diameter ratio >35, the one dimensional beam models and analytical solution techniques were employed to study the free vibration behaviour of CNTs using elastic modulus of 1 TPa and ∼0.34 nm effective wall thickness [5–9]. The free vibration of multi walled carbon nanotubes (MWCNTs) is investigated using Euler–Bernoulli and Timoshenko beam models depicting significant effect of shear deformation [5,6,8] and rotary inertia for the short CNTs. Based on the Euler–Bernoulli beam theory, the transverse free vibration frequencies of DWCNTs are shown to decrease with the increase in the axial compressive load [7]. However, the amplitude ratio for the inner and outer tubes was found to be independent of the axial compressive load.

The buckling of MWCNTs embedded in an elastic medium has been studied by representing each tube as Euler–Bernoulli [10] and Timoshenko [11] beams considering weak vdW interactions between adjacent tubes. The effect of vdW interaction was found to be significant for the greater half–wavelength to the outer most tube diameter ratio. The buckling of double walled carbon nanotubes (DWCNTs) used as a tip of an atomic force microscope with initial inclination and different lengths of the inner/outer tubes has been studied using Euler–Bernoulli beam model [12,13]. The critical buckling load was found to decrease with the increase in the initial inclination [12]. The critical axial compressive load of the longer tube was found to be greater if the shorter reinforcing tube was outside [13].

For the shorter CNTs with length to diameter ratio less than 35, the continuum shell models with the ability to capture the local deformations were found to be more accurate as compared to the beam models [14]. Among the continuum shell models, Liew and Wang [15] studied the wave propagation in CNTs (in–plane stiffness = 360 nN nm, wall thickness = 0.34 nm and bending rigidity = 2 nN nm) employing Love thin shell theory and Cooper–Naghdi thick shell theory and brought out the importance of the

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https://doi.org/10.1016/j.compstruc.2017.10.003
0045-7949/

latter for higher mode wave dispersion. Chowdhury et al. [16] studied the effect of clamping of one end of the constituent tubes on the free vibration frequencies of the five walled CNTs and observed that the rate of increase of the free vibration frequencies decreases with the increase in the number of the clamped constituent tubes with the greater sensitivity of the fundamental mode and the greater effect of clamping of the outermost tube as compared to inner tubes. The three dimensional closed form solutions were found to be almost close to those from beam models for length to diameter ratio >20 [17]. Strozzi et al. [18] employed Sanders–Koiter thin shell theory and Rayleigh–Ritz method for the free vibration analysis of SWCNTs with different boundary conditions.

The closed form solutions for buckling of SWCNTs/DWCNTs under axial compression [19,20] and torsion [21] predicted the negligible effect of vdW interactions on critical strain but significant effect of elastic medium especially for CNTs with relatively greater radius compared to the space between the tubes. With the decrease in the outermost tube radius to total thickness ratio of MWCNTs, the critical stress was found to increase and the effect of surrounding medium on buckling load was found to decrease [22]. The critical shear stress depicted the increasing trend with the tensile and decreasing one for the compressive axial load [23]. The effect of vdW interactions considered beyond the second neighbouring tube was found to be insignificant on the critical bucking load of MWCNTs [24]. The singular perturbation technique was employed to study the postbuckling behaviour of CNTs under different types of loading [25–28]. The postbuckling response under hydrostatic pressure was found to be stable for SWCNT and unstable for DWCNT. However, under axial compression and torsional loading, both the CNTs depicted unstable postbuckling path.

In the literature on the continuum modelling of CNTs, the bending stiffness is calculated using Young's modulus and wall thickness with significant scatter in the values. This arbitrariness of the extensional and bending stiffnesses can be eliminated using the molecular mechanics/dynamics simulations but at the cost of significantly greater computational requirements. The thickness and elastic properties of equivalent continuum model were proposed by comparing the flexural free vibration frequencies/in–plane force–strain relation for SLGSs and axial/torsional frequencies for CNTs using molecular mechanics simulation software TINKER and the closed form continuum mechanics solutions [29,30]. Reddy et al. [31] have performed the free vibration analysis of SWCNTs using continuum shell model and molecular mechanics simulation through Tersoff–Brenner potential and observed that the Young's modulus of ~3.5 TPa and wall thickness of ~0.066 nm yield the results close to those obtained from molecular mechanics simulations.

The investigation on the nonlinear tensile behaviour, elastic/plastic properties and buckling characteristics of CNTs using second generation REBO potential depicted significantly greater Young's modulus of SWCNTs as compared to MWCNTs [32] and the greater critical axial buckling strain for MWCNTs as compared to SWCNTs [33]. The MWCNTs with interlayer spacing <0.34 nm were found to be stiffer than MWCNTs with interlayer spacing equal to 0.34 nm [34]. The compressive critical strain of CNTs was found to be greater for zigzag configuration as compared to armchair whereas the critical torsional strain was found to be almost the same with the greater effect of temperature on the former [35,36].

To achieve the accuracy of the molecular mechanics simulations and the computational efficiency of continuum modelling, the multiscale approaches are employed for the atomistic systems with large number of atoms. In the multiscale modelling, the constitutive matrix calculated directly from molecular potential functions at atomic scale is used at the continuum level. The molecular model accounting for the bond interactions is coupled to continuum model through Cauchy–Born rule. The elastic properties of SWCNTs were estimated using the Tersoff–Brenner interatomic potential in conjunction with Cauchy–Born rule [37], higher order Cauchy–Born rule [38,39] and exponential Cauchy–Born rule [40]. The free vibration behaviour of SWCNTs was studied employing higher order Cauchy–Born rule, Tersoff–Brenner potential and moving Kriging meshless method [41]. The results were found to be in good agreement with molecular mechanics simulation. It may be noted that the convergence and accuracy of moving Kriging meshless method is shape parameter dependent [42,43]. The multiscale modelling in conjunction with the finite element based solution technique is expected to be computationally efficient, robust and suitable for solving the problems with different boundary conditions and involving nonlinearities [40]. Triangular facet shell finite element in the framework of exponential Cauchy–Born rule was employed to study the large deformation behaviour of CNTs by Arroyo and Belytschko [40,44]. In these studies, the analysis was performed in two steps: (i) mapping the graphene sheet to CNT and (ii) then prediction of deformation under applied load. This approach leads to the requirement of additional drilling degree of freedom resulting in increased computational time added with the requirement of transformation from local to global coordinate frame. This can be eliminated if CNT is modelled in cylindrical coordinate system. However, in cylindrical coordinate system, there may be membrane locking. The locking free finite element formulation in cylindrical coordinate system for CNT modelling based on multiscale approach has not been attempted in the literature. The computational efficiency can further be improved using higher order finite elements. Further, the quantitative effect of material and geometric nonlinearities on the postbuckling path has not been explicitly explored in the available literature.

The main aim of the present paper is to develop the locking free finite element formulation in cylindrical coordinate system for the modelling of CNTs based on multiscale approach and to characterise their dynamic and postbuckling behaviour incorporating material and geometric nonlinearities. The atomic interactions are modelled through Tersoff–Brenner potential. The four and eight noded Kirchhoff rectangular and improved discrete Kirchhoff quadrilateral (IDKQ) [45] finite elements are developed and assessed for their computational efficiency and accuracy for the free vibration frequencies of SWCNTs. To avoid the membrane locking, the circumferential strain is interpolated consistently using smoothed interpolation functions obtained through least square smoothing technique [46–48]. The other smoothing techniques to eliminate the locking in finite elements can also be employed [49–52]. The free vibration frequencies of first few modes obtained from multiscale shell model are compared with molecular mechanics simulations. For the dynamic response, governing equations are solved using Newmark's time integration technique and postbuckling path is traced using Newton–Raphson method in conjunction with adaptive displacement control [53,54].

2. Constitutive law

In the atomistic–continuum coupled framework, the bond vectors in deformed ($\mathbf{r}_{ij}$) and undeformed configurations ($\mathbf{r}^0_{ij}$) are related through the continuum deformation gradient ($\widetilde{\mathbf{F}}$) using Cauchy–Born rule as:

$$\mathbf{r}_{ij} = \widetilde{\mathbf{F}}\mathbf{r}^0_{ij} \tag{1}$$

Considering the effect of internal relaxation ($\boldsymbol{\eta}$), macroscopic Green–Lagrange strain ($\mathbf{E}$) and curvature ($\mathbf{K}$) tensors, the deformed bond length is given as [37,55]: