MULTISCALE MODELLING OF GRAPHENE SHEETS AND CARBON NANOTUBES

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by

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Certificate

This is to certify that the thesis entitled **"Multiscale Modelling of Graphene Sheets and Carbon Nanotubes"** being submitted by **Mr. Sandeep Singh** to the Indian Institute of Technology Delhi for the award of degree of **Doctor of Philosophy** in Applied Mechanics is a record of original, bonafide research work carried out by him under my supervision and guidance. The thesis work, in my opinion, has reached the requisite standard fulfilling the requirements for the degree of Doctor of Philosophy.

The results contained in this thesis have not been submitted in part or in full, to any other university or institute for the award of any degree or diploma.

Date: February ___, 2017

Place: New Delhi

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(Sandeep Singh)

Abstract

The multiscale modelling of graphene sheets and carbon nanotubes is computationally efficient and has almost the same accuracy as that of the atomistic simulation. It is concluded from the literature review that the nonlinear constitutive behaviour at finite strain and curvatures, nonlinear static/dynamic behaviour of graphene sheets including material and geometric nonlinearities have not been investigated. Further, there is a need to develop computationally efficient locking free finite element in cylindrical coordinate system for multiscale modelling of carbon nanotubes.

The present work deals with the multiscale modelling of the graphene sheets and carbon nanotubes in the finite element framework incorporating material and geometric nonlinearities through interatomic potential and strain–displacement relations, respectively. The deformations at atomic and continuum levels are coupled through Cauchy–Born rule including the effect of curvature tensor on the bond length. The nonlinear constitutive law is derived from the strain energy density function obtained through Tersoff–Brenner potential. The four noded Kirchhoff rectangular element is employed to discretise the graphene sheet at continuum level. The four/eight noded Kirchhoff rectangular and improved discrete Kirchhoff quadrilateral membrane inconsistent/consistent elements are developed and employed to discretise the carbon nanotubes.

The nonlinear static and dynamic response of graphene sheets under transverse and in– plane loading and buckling/postbuckling response of carbon nanotubes under axial compressive loading are investigated with/without material and geometric nonlinearities. The transverse bending response of graphene sheets depicts softening behaviour with the inclusion of material nonlinearity. The frequency response curves of graphene sheets,

obtained using shooting technique in conjunction with Newmark's time integration scheme, depict greater effect of geometric nonlinearity as compared to material nonlinearity for the loading parameters considered.

The investigation on free vibration and buckling characteristics of carbon nanotubes revealed that the consistent interpolation of transverse displacement in circumferential strain or quadratic interpolation of in–plane displacements significantly improves the convergence rate as compared to four noded inconsistent element. In order to trace equilibrium path with the presence of limit points for carbon nanotubes under axial compressive loading, Newton–Raphson method in conjunction with the adaptive displacement control and a computationally efficient asymptotic numerical method are employed. The asymptotic numerical method is directly applied to cubic nonlinear problem without converting it into quadratic form for the first time. The efficacy and accuracy of the asymptotic numerical method is investigated considering transverse bending of a plate, snap–through buckling of a cylindrical panel under central point load and bending/postbuckling of graphene sheets. The significant increase in the limit point load is observed with the inclusion of material nonlinearity due to hardening nature of constitutive law under compressive strains.

सारांश

ग्राफीन चादरों एवं कार्बन की अतिसूक्ष्म नलिकाओं का बहुपैमानीय प्रतिरूपण गणनात्मक द्रष्टि से तीव्र एवं परमाणवीय आकलन के लगभग समान है। इस विषय पर साहित्य समीक्षा करने पर पता चलता है कि ग्राफीन चादरों का अशून्य विकृति एवं वक्रता पर अरेखीय प्रतिबल–विकृति संबंध तथा अरेखीय स्थैतिक/गत्यात्मक व्यवहार, असमानुपातिक प्रतिबल–विकृति एवं विकृति–विस्थापन संबंधों के साथ अध्ययन नहीं किये गये हैं। इसके अतिरिक्त, कार्बन की अतिसूक्ष्म नलिकाओं का बहुपैमानीय प्रतिरूपण करने के लिए गणनात्मक द्रष्टि से तीव्र एवं अव्यवहारिक दृढ़ता मुक्त बेलनीय समन्वय में अल्पांशों के विकास क़ी जरुरत है।

वर्तमान लेखन, ग्राफीन चादरों एवं कार्बन की अतिसूक्ष्म नलिकाओं का बहुपैमानीय प्रतिरूपण अल्पांश विधि के ढांचे में अरेखीय प्रतिबल–विकृति एवं विकृति–विस्थापन संबंधों के साथ प्रस्तुत करता है। अरेखीय प्रतिबल–विकृति संबंध, टेरसॉफ–ब्रेनर अंतरपरमाणवीय स्थितिज ऊर्जा से व्युत्पन्न किया गया है। वक्रता का आणविक बंध लम्बाई पर प्रभाव के साथ परमाणवीय एवं सतत पैमानीय विस्थापनों को कौशी–बोर्न नियम के तहत संबंधित किया गया है। ग्राफीन चादरों को सतत पैमाने पर चार नोड वाले किरकोफ आयताकार अल्पांश से विभाजित किया गया है। चार/आठ नोड वाले किरकोफ आयताकार एवं उन्नत असतत किरकोफ चतुष्कोणीय संगत/असंगत मेम्ब्रेन विकृति अंतर्वेशन वाले अल्पांशों का विकास एवं उपयोग कार्बन की अतिसूक्ष्म नलिकाओं को विभाजित करने के लिए किया गया है।

ग्राफीन चादरों का अनुप्रस्थ एवं इन–प्लेन बलों के अधीन स्थैतिक एवं गत्यात्मक व्यवहार और कार्बन की अतिसूक्ष्म नलिकाओं का धुरी के समानान्तर बलों के अधीन बकलिंग/पोस्टबकलिंग व्यवहार रेखीय/अरेखीय प्रतिबल–विकृति एवं विकृति–विस्थापन संबंधों के साथ अध्ययन किया गया है। ग्राफीन चादरों का अनुप्रस्थ बलों के अधीन अरेखीय प्रतिबल–विकृति गुणधर्म नरम प्रकृति दर्शाता है। शूटिंग एवं न्यूमार्क की समय समाकलन विधियों के अनुपयोग से निकाले गये आवर्ती व्यवहार पर विकृति–विस्थापन संबंध की अरेखीयता का प्रभाव प्रतिबल–विकृति संबंध की अरेखीयता के प्रभाव से ज्यादा पाया गया है।

कार्बन की अतिसूक्षम नलिकाओं क़ी आज़ाद कम्पन एवं बकलिंग विशेषतायें दर्शाते हैं कि परिधीय विकृति में अनुप्रस्थ विस्थापन का संगत अथवा द्विघातीय अंतर्वेशन करने से अभिसरण दर चार नोड वाले असंगत अल्पांश से महत्वपूर्ण ढंग से बेहतर हुयी है। कार्बन की अतिसूक्ष्म नलिकाओं का धुरी के समानान्तर दाबक बलों के अधीन प्रतिबंध बिंदुओं वाले संतुलन पथ को निकालने के लिए अनुकूलक विस्थापन नियंत्रण के साथ न्यूटन–राफसेन एवं अभिकलनात्मकता की द्रष्टि से कुशल एसिम्पटोटिक न्यूमेरिकल तरीका अपनाया गया है। एसिम्पटोटिक न्यूमेरिकल तरीका त्रिघातीय अरेखीय समीकरण को सीधे तौर पर बिना द्विघातीय रूप में बदले ही पहली बार इस लेखन में इस्तेमाल किया है। एसिम्पटोटिक न्यूमेरिकल तरीके की क्षमता और कुशलता का निरूपण करने के लिए चादर का अनुप्रस्थ नमन, केन्द्रित बल के अधीन बेलनीय पैनल का स्नैप–थ्रू बकलिंग एंव ग्राफीन चादरों का नमन/पोस्टबकलिंग का अध्ययन किया गया है। दबावी विकृति के अधीन बढ़ती दृढ़ता वाले प्रतिबल–विकृति संबंध के प्रभाव से, प्रतिबंध बिन्दुयों के बल के परिमाण में महत्वपूर्ण ढंग से वृद्धि पायी गयी है।

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Nomenclature and Abbreviations

English Notations

$a,\ b$	:	Dimensions of the graphene sheet along x and y directions, respectively
a_i	:	Constants of Newmark's time integration scheme
$\tilde{a}$	:	Path parameter in asymptotic numerical method
$\mathbf{a}_1,\ \mathbf{a}_2$	:	Lattice vectors of the unit cell
$\mathbf{A},\ \mathbf{B},\ \mathbf{D}$	:	Tangent extensional, bending–extension coupling and bending stiffness coefficient matrices, respectively
$\mathbf{B}_L,\ \mathbf{B}_{NL}$	:	Linear and nonlinear strain/curvature–displacement matrix, respectively
$\mathbf{C}_h$	:	Chiral vector
$\mathbf{C}_e,\ \mathbf{C}$	:	Elemental and global damping matrix
$\mathbf{d}_e,\ \dot{\mathbf{d}}_e,\ \ddot{\mathbf{d}}_e$	:	Elemental displacement, velocity and acceleration vector
$\mathbf{d},\ \dot{\mathbf{d}},\ \ddot{\mathbf{d}}$	:	Global displacement, velocity and acceleration vector
$\bar{\mathbf{d}}_w,\ \tilde{\mathbf{d}}_w$	:	Vector of transverse and rotational degrees of freedom for Kirchhoff rectangular and IDKQ elements, respectively
$\bar{\mathbf{D}}$	:	Tangent constitutive matrix

$D_0,\ S,\ R_e,$ $a_{0,}\ c_0,\ d_0$	:	Parameters of interatomic potential function
$\tilde{\mathbf{E}},\ \mathbf{E}$	:	Green–Lagrange strain tensor
E_1	:	Young's Modulus along x direction
$\mathbf{F}_e,\ \mathbf{F}$	:	Elemental and global external load vectors
$\mathbf{F}_{ine},\ \mathbf{F}_{in}$	:	Elemental and global internal load vectors
$\mathbf{F}_e^b$	:	Force vector due to stress and moment resultants along the boundary of an element
$\mathbf{F}_0$	:	Global external load vector corresponding to unit load
$\tilde{\mathbf{F}}$	:	Deformation gradient tensor
h	:	Thickness of the graphene sheet along z direction
$\mathbf{H}$	:	Transverse displacement interpolation vector
$\mathbf{K}_{Te},\ \mathbf{K}_T$	:	Elemental and global tangent stiffness matrices
$\mathbf{K}_{Ge},\ \mathbf{K}_G$	:	Elemental and global geometric stiffness matrices
$\mathbf{K}_L$	:	Linear global stiffness matrix
$\tilde{\mathbf{K}}_G$	:	Global geometric stiffness matrix due to unit axial force $\bar{S}_{xx}$ = 1 nN/nm at $x = L$
$\mathbf{K}_1,\ \mathbf{K}_2,\ \mathbf{K}_3$	:	Restoring forces linearly, quadratically and cubically dependent on displacement vector
$\tilde{\mathbf{K}},\ \mathbf{K}$	:	Curvature tensor
$l_x,\ l_y$	:	Length of the element along x and y directions

L, D, R	:	Length, diameter and radius of the nanotube, respectively
$m,\ n$	:	Integer numbers
m_c	:	Mass of the carbon atom
M	:	Order of expansion in asymptotic numerical method
$\tilde{\mathbf{M}}_e,\ \tilde{\mathbf{M}}$	:	Elemental and global mass matrices
$\mathbf{M}^m,\ \mathbf{d}^m,$ $\tilde{\mathbf{d}}^m,\ \mathbf{F}^m$	:	Diagonal mass matrix, global degrees of freedom vector, modal amplitude vector and external load vector in MM simulation, respectively
$\mathbf{n}_{ij}^0$	:	Unit vector along the undeformed bond vector
$N_i,\ H_i,\ \bar{H}_i,$ $\tilde{G}_i,\ \tilde{H}_i$	:	Interpolation functions used in finite element interpolation
$Q,\ \bar{S}_{xx}$	:	Transverse/radial and in–plane loads
$r_{ij},\ r^0$	:	Deformed and undeformed bond lengths
$\mathbf{r}_{ij},\ \mathbf{r}_{ij}^0$	:	Deformed and undeformed bond vectors
$\mathbf{S},\ \mathbf{M}$	:	Second Piola–Kirchhoff stress and moment resultant tensors
$\tilde{T},\ \Phi,\ \tilde{W}$	:	Kinetic energy, strain energy and virtual work of external loads
$T,\ t$	:	Time period and any arbitrary time
$u,\ v,\ w$	:	Displacements along x, y and z directions, respectively
$\mathbf{U}$	:	Interpolation matrix of displacement field

V	:	Interatomic potential function between two atoms
W	:	Strain energy per unit area or strain energy density function

Greek Notations

β	:	Chiral angle
$\beta_0,\ \delta$	:	Parameters of interatomic potential function
$\boldsymbol{\eta}$	:	Internal relaxation vector
$\tilde{\boldsymbol{\eta}}$	:	State vector consisting of displacement and velocity vectors
ε_d	:	Infinitesimal number
Γ, Γ_e	:	Total surface area and area of a finite element
λ	:	Load multiplier
$\tilde{\lambda},\ \tilde{\delta}$	:	Constants of Newmark's time integration scheme
υ_{12}	:	Poisson's ratio in *x*–*y* plane
$\omega_F,\ \omega_{ni}$	:	Forcing frequency and natural frequency of *i*th mode
Ω	:	Area of the unit cell of the graphene sheet
ρ	:	Area mass density of a unit cell of graphene sheet
θ_{ijk}	:	Angle between bonds

Abbreviations

ANM	:	Asymptotic numerical method
AFM	:	Atomic force microscope
CNT	:	Carbon nanotube
DFT	:	Density functional theory
DLGS	:	Double layered graphene sheet
DWCNT	:	Double walled carbon nanotube
FFT	:	Fast Fourier transform
GS	:	Graphene sheet
IDKQ	:	Improved discrete Kirchhoff quadrilateral
MLGS	:	Multi layered graphene sheet
MM/MD	:	Molecular mechanics/ Molecular dynamics
MNL	:	Material Nonlinearity
MWCNT	:	Multi walled carbon nanotube
REBO	:	Reactive empirical bond order
SLGS	:	Single layer graphene sheet
SWCNT	:	Single walled carbon nanotube
UFF	:	Universal force field
vdW	:	Van der Waals