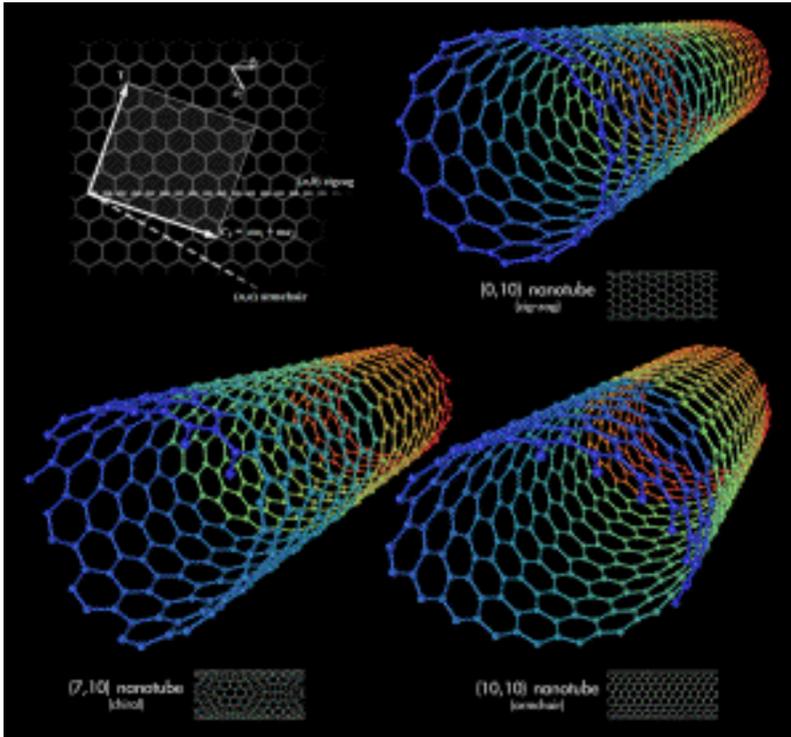


Buckling of Carbon Nanotubes

Part 1: Background from <http://www.mc2quantum.com/2009/07/carbon-nanotube/>



Carbon nanotubes (CNTs) are molecular-scale tubes of graphitic carbon with outstanding properties. They are among the stiffest and strongest fibres known, and have remarkable electronic properties and many other unique characteristics. For these reasons they have attracted huge academic and industrial interest, with thousands of papers on nanotubes being published every year. Commercial applications have been rather slow to develop, however, primarily because of the high production costs of the best quality nanotubes. Carbon Nanotube 3D

Carbon nanotubes are allotropes of carbon with a cylindrical nanostructure. Nanotubes have been constructed with length-to-diameter ratio of up to 28,000,000:1, which is significantly larger than any other material. These cylindrical carbon molecules have novel properties that make them potentially useful in many applications in nanotechnology, electronics, optics and other fields of materials science, as well as potential uses in architectural fields. They exhibit extraordinary strength and unique electrical properties, and are efficient conductors of heat. Their final usage, however, may be limited by their potential toxicity.

Nanotubes are members of the fullerene structural family, which also includes the spherical buckyballs. The ends of a nanotube might be capped with a hemisphere of the buckyball structure. Their name is derived from their size, since the diameter of a nanotube is on the order of a few nanometers (approximately 1/50,000th of the width of a human hair), while they can be up to several millimeters in length (as of 2008). Nanotubes are categorized as single-walled nanotubes (SWNTs) and multi-walled nanotubes (MWNTs).

The nature of the bonding of a nanotube is described by applied quantum chemistry, specifically, orbital hybridization. The chemical bonding of nanotubes is composed entirely of sp^2 bonds, similar to those of graphite. This bonding structure, which is stronger than the sp^3 bonds found in diamonds, provides the molecules with their unique strength. Nanotubes naturally align themselves into "ropes" held together by Van der Waals forces. Under high pressure, nanotubes can merge together, trading some sp^2 bonds for sp^3 bonds, giving the possibility of producing strong, unlimited-length wires through high-pressure nanotube linking.

Strength:

Carbon nanotubes are the strongest and stiffest materials yet discovered in terms of tensile strength and elastic modulus respectively. This strength results from the covalent sp^2 bonds formed between the individual carbon atoms. In 2000, a multi-walled carbon nanotube was tested to have a tensile strength of 63 gigapascals (GPa). (This, for illustration, translates into the ability to endure weight of 6300 kg on a cable with cross-section of 1 mm².) Since carbon nanotubes have a low density for a solid of 1.3-1.4 g/cm³, its specific strength of up to 48,000 kN·m/kg is the best of known materials, compared to high-carbon steel's 154 kN·m/kg.

Under excessive tensile strain, the tubes will undergo plastic deformation, which means the deformation is permanent. This deformation begins at strains of approximately 5% and can increase the maximum strain the tubes undergo before fracture by releasing strain energy.

CNTs are not nearly as strong under compression. Because of their hollow structure and high aspect ratio, they tend to undergo buckling when placed under compressive, torsional or bending stress.

Kinetic Types of Carbon Nanotubes:

Multi-walled nanotubes, multiple concentric nanotubes precisely nested within one another, exhibit a striking telescoping property whereby an inner nanotube core may slide, almost without friction, within its outer nanotube shell thus creating an atomically perfect linear or rotational bearing. This is one of the first true examples of molecular nanotechnology, the precise positioning of atoms to create useful machines. Already this property has been utilized to create the world's smallest rotational motor. Future applications such as a gigahertz mechanical oscillator are also envisaged.

Electrical:

Because of the symmetry and unique electronic structure of graphene, the structure of a nanotube strongly affects its electrical properties. For a given (n,m) nanotube, if $n = m$, the nanotube is metallic; if $n - m$ is a multiple of 3, then the nanotube is semiconducting with a very small band gap, otherwise the nanotube is a moderate semiconductor. Thus all armchair ($n=m$) nanotubes are metallic, and nanotubes (5,0), (6,4), (9,1), etc. are semiconducting. In theory, metallic nanotubes can carry an electrical current density of 4×10^9 A/cm² which is more than 1,000 times greater than metals such as copper.

Thermal:

All nanotubes are expected to be very good thermal conductors along the tube, exhibiting a property known as

_ballistic conduction, _ but good insulators laterally to the tube axis. It is predicted that carbon nanotubes will be able to transmit up to 6000 watts per meter per Kelvin at room temperature; compare this to copper, a metal well-known for its good thermal conductivity, which transmits 385 watts per meter per K. The temperature stability of carbon nanotubes is estimated to be up to 2800oC in vacuum and about 750oC in air.

Part 2: Selected publications about buckling of carbon nanotubes

Carbon Nanotubes and Nanosensors: Vibrations, Buckling, and Ballistic Impact

Isaac Elishakoff, *Florida Atlantic University, USA* Demetris Pentaras, *The Cyprus University of Technology, Cyprus* Kevin Dujat and Simon Bucas, *IFMA – French Institute for Advanced Mechanics, France* Claudia Versaci and Giuseppe Muscolino, *University of Messina, Italy* Joel Storch, *Touro College, USA* Noël Challamel, *INSA de Rennes, France* Toshiaki Natsuki, *Shinsu University, Japan* Yingyan Zhang, *University of Western Sydney, Australia* Chien Ming Wang, *National University of Singapore, Singapore* Guillaume Ghyselinck, *Ecole des Mines d'Alès, France*
ISBN: 9781848213456, December 2011, Hardback, 448 pp.

Description

The main properties that make carbon nanotubes (CNTs) a promising technology for many future applications are: extremely high strength, low mass density, linear elastic behavior, almost perfect geometrical structure, and nanometer scale structure. Also, CNTs can conduct electricity better than copper and transmit heat better than diamonds. Therefore, they are bound to find a wide, and possibly revolutionary use in all fields of engineering. The interest in CNTs and their potential use in a wide range of commercial applications; such as nanoelectronics, quantum wire interconnects, field emission devices, composites, chemical sensors, biosensors, detectors, etc.; have rapidly increased in the last two decades. However, the performance of any CNT-based nanostructure is dependent on the mechanical properties of constituent CNTs. Therefore, it is crucial to know the mechanical behavior of individual CNTs such as their vibration frequencies, buckling loads, and deformations under different loadings. This title is dedicated to the vibration, buckling and impact behavior of CNTs, along with theory for carbon nanosensors, like the Bubnov-Galerkin and the Petrov-Galerkin methods, the Bresse-Timoshenko and the Donnell shell theory.

Contents

1. Introduction. 2. Fundamental Natural Frequencies of Double-Walled Carbon Nanotubes. 3. Free Vibrations of the Triple-Walled Carbon Nanotubes. 4. Exact Solution for Natural Frequencies of Clamped-Clamped Double-Walled Carbon Nanotubes. 5. Natural Frequencies of Carbon Nanotubes Based on a Consistent Version of Bresse-Timoshenko Theory. 6. Natural Frequencies of Double-Walled Carbon Nanotubes Based on Donnell Shell Theory. 7. Buckling of a Double-Walled Carbon Nanotube. 8. Ballistic Impact on a Single-Walled Carbon Nanotube. 9. Clamped-Free Double-Walled Carbon Nanotube-Based Mass Sensor. 10. Some Fundamental Aspects of Non-local Beam Mechanics for Nanostructures Applications. 11. Surface Effects on the Natural Frequencies of Double-Walled Carbon Nanotubes. 12. Summary and Directions for Future Research.

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“Recent Studies on Buckling of Carbon Nanotubes”, Appl. Mech. Rev., Vol. 63, No. 3, May 2010, 030804 (18 pages), doi:10.1115/1.4001936

ABSTRACT: This paper reviews recent research studies on the buckling of carbon nanotubes. The structure and properties of carbon nanotubes are introduced to the readers. The various buckling behaviors exhibited by carbon nanotubes are also presented herein. The main factors, such as dimensions, boundary conditions, temperature, strain rate, and chirality, influencing the buckling behaviors are also discussed, as well as a brief introduction of the two most used methods for analyzing carbon nanotubes, i.e., continuum models and atomistic simulations. Summary and recommendations for future research are also given. Finally, a large body of papers is given in the reference section. It is hoped that this paper provides current knowledge on the buckling of carbon nanotubes, reviews the computational methods for determining the buckling loads, and inspires researchers to further investigate the buckling properties of carbon nanotubes for practical applications.

B. I. Yakobson, C. J. Brabec and J. Bernholc (Department of Physics, North Carolina State University, Raleigh, North Carolina 27695), **“Nanomechanics of Carbon Tubes: Instabilities beyond Linear Response”**, Phys. Rev. Lett. Vol. 76, pp. 2511–2514 (1996), doi: 10.1103/PhysRevLett.76.2511

ABSTRACT: Carbon nanotubes subject to large deformations reversibly switch into different morphological patterns. Each shape change corresponds to an abrupt release of energy and a singularity in the stress-strain curve. These transformations, simulated using a realistic many-body potential, are explained by a continuum shell model. With properly chosen parameters, the model provides a remarkably accurate “roadmap” of nanotube behavior beyond Hooke's law.

Wang, C.Y., Zhang, Y.Y., Wang, C.M. and Tan, V.B.C., **“Buckling of Carbon Nanotubes: A Literature Survey”**, Journal of Nanoscience and Nanotechnology, Vol. 7, No. 12, December 2007 , pp. 4221-4247, doi: 10.1166/jnn.2007.924

ABSTRACT: This survey paper comprises 5 sections. In Section 1, the reader is introduced to the world of carbon nanotubes where their structural form and properties are highlighted. Section 2 presents the various buckling behaviors exhibited by carbon nanotubes that are discovered by carbon nanotube researchers. The main factors, such as dimensions, boundary conditions, temperature, strain rate and chirality, influencing the buckling behaviors are discussed in Section 3. Section 4 presents the continuum models, atomistic simulations and experimental techniques in studying the buckling phenomena of carbon nanotubes. A summary as well as recommendations for future research are given in Section 5. Finally a large body of papers, over 200, is given in the reference section. It is hoped that this survey paper will provide the foundation knowledge on carbon nanotube buckling and inspire researchers to advance the modeling, simulation and design of carbon nanotubes for practical applications.

Harik, V. M. ; Gates, T. S. ; Nemeth, M. P., “Applicability of the Continuum-shell Theories to the Mechanics of Carbon Nanotubes”, Institute For Computer Applications In Science And Engineering Hampton VA, Accession Number : ADA401873, Handle / proxy Url <http://handle.dtic.mil/100.2/ADA401873> . , April 2002

ABSTRACT: Validity of the assumptions relating the applicability of continuum shell theories to the global mechanical behavior of carbon nanotubes is examined. The present study focuses on providing a basis that can be used to qualitatively assess the appropriateness of continuum-shell models for nanotubes. To address the effect of nanotube structure on their deformation, all nanotube geometries are divided into four major classes that require distinct models. Criteria for the applicability of continuum models are presented. The key parameters that control the buckling strains and deformation modes of these classes of nanotubes are determined. In an analogy with continuum mechanics, mechanical laws of geometric similitude are presented. A parametric map is constructed for a variety of nanotube geometries as a guide for the applicability of different

models. The continuum assumptions made in representing a nanotube as a homogeneous thin shell are analyzed to identify possible limitations of applying shell theories and using their bifurcation-buckling equations at the nano-scale.

C. Y. Wang, C. Q. Ru and A. Mioduchowski (Department of Mechanical Engineering, 4-9 Mechanical Engineering Bldg., University of Alberta, Edmonton, Alberta., Canada T6G 2G8), "Axially compressed buckling of pressured multiwall carbon nanotubes", *International Journal of Solids and Structures*, Vol. 40, No.15, July 2003, pp. 3893-3911, doi:10.1016/S0020-7683(03)00213-0

ABSTRACT: This paper studies axially compressed buckling of an individual multiwall carbon nanotube subjected to an internal or external radial pressure. The emphasis is placed on new physical phenomena due to combined axial stress and radial pressure. According to the radius-to-thickness ratio, multiwall carbon nanotubes discussed here are classified into three types: thin, thick, and (almost) solid. The critical axial stress and the buckling mode are calculated for various radial pressures, with detailed comparison to the classic results of singlelayer elastic shells under combined loadings. It is shown that the buckling mode associated with the minimum axial stress is determined uniquely for multiwall carbon nanotubes under combined axial stress and radial pressure, while it is not unique under pure axial stress. In particular, a thin N-wall nanotube (defined by the radius-to-thickness ratio larger than 5) is shown to be approximately equivalent to a single layer elastic shell whose effective bending stiffness and thickness are N times the effective bending stiffness and thickness of singlewall carbon nanotubes. Based on this result, an approximate method is suggested to substitute a multiwall nanotube of many layers by a multilayer elastic shell of fewer layers with acceptable relative errors. Especially, the present results show that the predicted increase of the critical axial stress due to an internal radial pressure appears to be in qualitative agreement with some known results for filled singlewall carbon nanotubes obtained by molecular dynamics simulations.

C. Y. Wang, C. Q. Ru, and A. Mioduchowski (Department of Mechanical Engineering, University of Alberta, Edmonton T6G 2G8, Canada), "Applicability and Limitations of Simplified Elastic Shell Equations for Carbon Nanotubes", *J. Appl. Mech.*, Vol. 71, No. 5, September 2004, pp. 622 – 631, doi:10.1115/1.1778415

ABSTRACT: This paper examines applicability and limitations of simplified models of elastic cylindrical shells for carbon nanotubes. The simplified models examined here include Donnell equations and simplified Flugge equations characterized by an uncoupled single equation for radial deflection. These simplified elastic shell equations are used to study static buckling and free vibration of carbon nanotubes, with detailed comparison to exact Flugge equations of cylindrical shells. It is shown that all three elastic shell models are in excellent agreement (with relative errors less than 5%) with recent molecular dynamics simulations for radial breathing vibration modes of carbon nanotubes, while reasonable agreements for various buckling problems have been reported previously for Donnell equations. For general cases of buckling and vibration, the results show that the simplified Flugge model, which retains mathematical simplicity of Donnell model, is consistently in better agreement with exact Flugge equations than Donnell model, and has a significantly enlarged range of applicability for carbon nanotubes. In particular, the simplified Flugge model is applicable for carbon nanotubes (with relative errors around 10% or less) in almost all cases of physical interest, including some important cases in which Donnell model results in much larger errors. These results are significant for further application of elastic shell models to carbon nanotubes because simplified shell models, characterized by a single uncoupled equation for radial deflection, are particularly useful for multiwall carbon nanotubes of large number of layers.

J. G. Simmonds (Department of Civil Engineering, University of Virginia, Charlottesville, VA 22904), "Discussion: "Applicability and Limitations of Simplified Elastic Shell Equations for Carbon Nanotubes"

(Wang, C. Y., Ru, C. Q., and Mioduchowski, A., 2004, ASME J. Appl. Mech., 71, pp. 622–631), J. Appl. Mech., Vol. 72, No. 6, November 2005, 981 (1 pages) doi:10.1115/1.2040451

C.Y. Wang and A. Mioduchowski (Department of Mechanical Engineering, University of Alberta, Edmonton T6G 2G8, Canada), “The effect of dimensional factors on buckling of multiwall carbon nanotubes”, Journal of Applied Physics, Vol. 101, No. 1, June 2009, pp. 014306 – 014306-12, doi: 10.1063/1.2403865

ABSTRACT: Based on a multiple-shell model, a comprehensive investigation has been performed on the effect of three dimensional factors, i.e., aspect ratio, the innermost radius, and the number of layers, on buckling behavior of multiwall carbon nanotubes (MWCNTs) under axial compression or radial pressure. In contrast to previous shell models, which use the single Donnell equation [Wang et al, ASME J. Appl. Mech. 71, 622 (2004)] and thus are only adequate for buckling of MWCNTs of relatively small aspect ratio (e.g., not larger than 10), the present shell model based on the simplified Flugge equation [Wang et al, ASME J. Appl. Mech. 71, 622 (2004)] allows for the study of buckling behavior of MWCNTs without any limitation on their aspect ratios. In addition, the pressure dependence of the interlayer van der Waals interaction coefficient (defined as the second derivative of the interlayer potential energy-interlayer spacing relation) has been considered for pressure-induced buckling of MWCNTs. The relevance of the present shell model for buckling of MWCNTs has been confirmed by the good agreement between the present shell model and available discrete models or experiments. Here, distinct buckling behaviors under axial compression or radial pressure are identified for long and short MWCNTs, separated by a certain critical value of aspect ratio. On the other hand, while the critical buckling load usually changes monotonically with the innermost radius an optimum value of the number of layers associated with the maximum critical buckling pressure is obtained for MWCNTs under radial pressure. In particular, the present shell model shows that the three dimensional factors effecting buckling of MWCNTs are generally interacting with, rather than being independent of, one another.

Waters, J. F., Guduru, P. R., Jouzi, M., Xu, J. M., Hanlon, T. and Suresh, S. (Division of Engineering, Brown University, Providence, Rhode Island 02912), “Shell buckling of individual multiwalled carbon nanotubes using nanoindentation”, Applied Physics Letters, Vol. 87, No. 10, September 2005

ABSTRACT: Although the mechanical behavior of carbon nanotubes has been studied extensively in recent years, very few experimental results exist on the shell buckling of nanotubes, despite its fundamental importance in nanotube mechanics and applications. Here we report an experimental technique in which individual multiwalled carbon nanotubes were axially compressed using a nanoindenter and the critical shell-buckling load was measured. The results are compared with predictions of existing continuum theories, which model multiwalled carbon nanotubes as a collection of single-walled shells, interacting through van der Waals forces. The theoretical models significantly underpredict the experimental buckling load.

J F Waters , P R Guduru , J M Xu, “Nanotube mechanics - Recent progress in shell buckling mechanics and quantum electromechanical coupling”, Composites Science and Technology 66 (2006)

Abu-Salih, Samy; Moussa, Walied A., “Electromechanical Buckling and Postbuckling of Micro Cylindrical Shells”, Journal of Computational and Theoretical Nanoscience, Vol. 5, No. 10, October 2008 , pp. 2045-2053(9), doi: 10.1166/jctn.2008.1012

ABSTRACT: In this work the electromechanical buckling and postbuckling responses of a circular cylindrical shallow shell are analyzed. The cylindrical shell is subjected to a radial axi-symmetric electrostatic field that is generated by setting voltage difference between an exterior elastic thin shallow cylinder and an inner infinitely stiff solid cylinder. The nonlinear prebuckling state of the cylinder is considered in order to increase the accuracy of the analysis. The prebuckling, buckling and postbuckling states are solved by implementing the

perturbation asymptotic approach. The critical electromechanical buckling voltage and the stability of the postbuckling states are solved for a wide range value of the geometrical parameters of the elastic shell, such as radius-thickness ratio, the radius-length ratio and the ratio between the radius of the interior stiff cylinder and the exterior cylindrical shell. The numerical results show that the initial electromechanical postbuckling of the shell is unstable for all the considered range of parameters.

Markus J. Buehler, Yong Kong, and Huajian Gao (Max Planck Institute for Metals Research, Heisenbergstr. 3, 70569 Stuttgart, Germany), "Deformation Mechanisms of Very Long Single-Wall Carbon Nanotubes Subject to Compressive Loading", *ASME J. Eng. Mater. Technol.*, Vol. 126, No. 3, July 2004, pp. 245 – 249, doi:10.1115/1.1751181

ABSTRACT: Author(s):

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We report atomistic studies of single-wall carbon nanotubes with very large aspect ratios subject to compressive loading. These long tubes display significantly different mechanical behavior than tubes with smaller aspect ratios. We distinguish three different classes of mechanical response to compressive loading. While the deformation mechanism is characterized by buckling of thin shells in nanotubes with small aspect ratios, it is replaced by a rod-like buckling mode above a critical aspect ratio, analogous to the Euler theory in continuum mechanics. For very large aspect ratios, a nanotube is found to behave like a flexible macromolecule which tends to fold due to vdW interactions between different parts of the carbon nanotube. This suggests a shell-rod-wire transition of the mechanical behavior of carbon nanotubes with increasing aspect ratios. While continuum mechanics concepts can be used to describe the first two types of deformation, statistical methods will be necessary to describe the dynamics of wire-like long tubes.

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"Molecular Scale Buckling Mechanics in Individual Aligned Single-Wall Carbon Nanotubes on Elastomeric Substrates", *Nano Lett.*, 2008, 8 (1), pp 124–130, doi: 10.1021/nl072203s

ABSTRACT: We have studied the scaling of controlled nonlinear buckling processes in materials with dimensions in the molecular range (i.e., about 1 nm) through experimental and theoretical studies of buckling in individual single-wall carbon nanotubes on substrates of poly(dimethylsiloxane). The results show not only the ability to create and manipulate patterns of buckling at these molecular scales, but also, that analytical continuum mechanics theory can explain, quantitatively, all measurable aspects of this system. Inverse calculation applied to measurements of diameter-dependent buckling wavelengths yields accurate values of the

Young's moduli of individual SWNTs. As an example of the value of this system beyond its use in this type of molecular scale metrology, we implement parallel arrays of buckled SWNTs as a class of mechanically stretchable conductor.

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“Buckling Analyses of Double-Wall Carbon Nanotubes: A Shell Theory Based on the Interatomic Potential”, *J. Appl. Mech.*, Vol. 77, No. 6, November 2010, 061016 (6 pages), doi:10.1115/1.4001286

ABSTRACT: Based on the finite-deformation shell theory for carbon nanotubes established from the interatomic potential and the continuum model for van der Waals (vdW) interactions, we have studied the buckling of double-walled carbon nanotubes subjected to compression or torsion. Prior to buckling, the vdW interactions have essentially no effect on the deformation of the double-walled carbon nanotube. The critical buckling strain of the double-wall carbon nanotubes is always between those for the inner wall and for the outer wall, which means that the vdW interaction decelerates buckling of one wall at the expenses of accelerating the buckle of the other wall.

V. Chiroiu, L. Munteanu...”Evaluation of the Toupin-Mindlin theory for predicting the size effects in the buckling of the carbon nanotubes”, *Computers, Materials, &... 2010* (techscience.com), Tech Science Press CMC, vol. 16, No. 1, 2010, pp. 75-100 (pdf file not available, no abstract, possibly incomplete author citation)

A. Sears and R. C. Batra (Department of Engineering Science and Mechanics, MC 0219 Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061, USA), “Macroscopic properties of carbon nanotubes from molecular-mechanics simulations”, *Phys. Rev. B*, Vol. 69, 235406 (2004) [10 pages], doi: 10.1103/PhysRevB.69.235406

ABSTRACT: Results of molecular-mechanics simulations of axial and torsional deformations of a single wall carbon nanotube are used to find Young's modulus, the shear modulus, and the wall thickness of an equivalent continuum tube made of a linear elastic isotropic material. These values are used to compare the response of the continuum tube in bending and buckling with that obtained from the molecular mechanics simulations. It is found that the strain energy of bending deformation computed from the Euler-Bernoulli beam theory matches well with that obtained from the molecular-mechanics simulations. The molecular-mechanics predictions of the critical strains for axial buckling and shell wall buckling do not match well with those derived from the Euler buckling formula and the Donnell shell theory.

A. Sears and R. C. Batra (Department of Engineering Science and Mechanics, M/C 0219, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061, USA), “Buckling of multiwalled carbon nanotubes under axial compression”, *Phys. Rev. B*, Vol. 73, 085410 (2006) [11 pages], doi: 10.1103/PhysRevB.73.085410

ABSTRACT: Buckling of single-walled and multiwalled carbon nanotubes (SWNTs and MWNTs, respectively) due to axial compressive loads has been studied by molecular mechanics simulations, and results compared with those from the analysis of equivalent continuum structures using Euler buckling theory and the finite element method. It is found that a MWNT of large aspect ratio (length/diameter) buckles as a column with axial strain at buckling given reasonably well by the Euler buckling theory applied to the equivalent continuum structure. However, a MWNT of low aspect ratio buckles in shell wall buckling mode with the axial strain at buckling corresponding to the highest axial strain at buckling of one of its constituent SWNTs. A finite element model has been developed that simulates van der Waals forces by truss elements connecting nodes on adjacent

walls of a MWNT; the axial strain at buckling from it is close to that obtained from the MM simulations but the two sets of mode shapes are different.

Chun Li and Wanlin Guo (Institute of Nanoscience, Nanjing University of Aeronautics and Astronautics, 29 Yudao Street, Nanjing, 210016, China), “Continuum Mechanics Simulation of Post-buckling of Single-Walled Nanotubes”, *International Journal of Nonlinear Sciences and Numerical Simulation*, Vol. 4, No. 4, pp. 387–394, doi: 10.1515/IJNSNS.2003.4.4.387

ABSTRACT: Large deformation behavior and post-buckling modes of single-walled carbon nanotubes are studied numerically by using traditional continuum shell theory and eigenvalue buckling methodology with elasticity parameters obtained by atomistic methods incorporated. Comparison with molecular mechanics and an atomistic-based continuum membrane method shows that the continuum shell theory is convenient and efficient in predicting the post-buckling behavior of the nanotubes subjected to axial compression, torsion and bend loads, providing that the elasticity parameters of the tube are obtained from atomistic theory. Higher-order buckling modes, which are difficult to be obtained by molecular mechanics, have been analyzed as well.

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(5) Department of Naval Architecture, Dalian University of Technology, People’s Republic of China

“Assessment of continuum mechanics models in predicting buckling strains of single-walled carbon nanotubes”, *Nanotechnology* Vol. 20, No. 39, 2009, 395707, doi: 10.1088/0957-4484/20/39/395707

ABSTRACT: This paper presents an assessment of continuum mechanics (beam and cylindrical shell) models in the prediction of critical buckling strains of axially loaded single-walled carbon nanotubes (SWCNTs). Molecular dynamics (MD) simulation results for SWCNTs with various aspect (length-to-diameter) ratios and diameters will be used as the reference solutions for this assessment exercise. From MD simulations, two distinct buckling modes are observed, i.e. the shell-type buckling mode, when the aspect ratios are small, and the beam-type mode, when the aspect ratios are large. For moderate aspect ratios, the SWCNTs buckle in a mixed beam–shell mode. Therefore one chooses either the beam or the shell model depending on the aspect ratio of the carbon nanotubes (CNTs). It will be shown herein that for SWCNTs with long aspect ratios, the local Euler beam results are comparable to MD simulation results carried out at room temperature. However, when the SWCNTs have moderate aspect ratios, it is necessary to use the more refined nonlocal beam theory or the Timoshenko beam model for a better prediction of the critical strain. For short SWCNTs with large diameters, the nonlocal shell model with the appropriate small length scale parameter can provide critical strains that are in good agreement with MD results. However, for short SWCNTs with small diameters, more work has to be done to refine the nonlocal cylindrical shell model for better prediction of critical strains.

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“Stability analysis of carbon nanotubes via continuum models”, *Smart Mater. Struct.*, Vol. 14, 2005, 281

doi: 10.1088/0964-1726/14/1/029

ABSTRACT: This paper presents the research on the stability analysis of carbon nanotubes (CNTs) via elastic continuum beam and shell models. The estimation of the flexural stiffness of a single-walled nanotube (SWNT) via the elastic beam model is proposed based on the postulate analyzed and provided in the paper. The validation of the stiffness is conducted with the ab initio calculations of the vibration of a SWNT. Based on the stiffness proposed, the stability analysis of CNTs is further conducted and validated with the well-cited research results by Yakobson and his collaborators. In addition, more predictions of various buckling phenomena of carbon nanotubes by beam and shell models are provided and studied. Finally, the kink phenomenon in a SWNT under pure bending is discussed via the continuum model. It is hoped that this paper will pave the way toward a better understanding of the application of continuum models in the stability and dynamics analysis of carbon nanotubes.

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“Small scale effect on elastic buckling of carbon nanotubes with nonlocal continuum models”, *Physics Letters A*, Vol. 357, No. 2, September 2006, pp. 130-135, doi:10.1016/j.physleta.2006.04.026

ABSTRACT: Nonlocal elastic beam and shell models are developed and applied to investigate the small scale effect on buckling analysis of carbon nanotubes (CNTs) under compression. General and explicit solutions are derived and expressed in terms of the solutions via local or classical elastic models, in which the scale effect is not accounted, to reveal the small scale effect on CNTs buckling results. The dependence of the scale effect with respect to the length, radius, and buckling modes of CNTs is clearly established and observed from the universal solutions derived in the manuscript. It is clearly seen from the results that the buckling solutions for CNTs via local continuum mechanics are overestimated and hence the scale effect is indispensable in providing more accurate results for mechanical behaviors of CNTs via continuum mechanics.

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“Torsional buckling of carbon nanotubes”, *Physics Letters A*, Vol. 367, Nos. 1-2, July 2007, pp.135-139, doi:10.1016/j.physleta.2007.02.099

ABSTRACT: Continuum mechanics models for the torsional buckling of carbon nanotubes (CNTs) are developed in the Letter. The applicability of these models is investigated for CNTs with different aspect ratios. In particular, molecular dynamics simulations are conducted to verify the feasibility of the models for moderately long CNTs.

Q. Wang (Department of Mechanical and Manufacturing Engineering, University of Manitoba, Winnipeg, Manitoba R3T 5V6, Canada), “Instability analysis of double-walled carbon nanotubes subjected to axial compression”, *Journal of Applied Physics*, Vol. 104, No. 3, 2008, pp. 036102-036102-3, doi: 10.1063/1.2955740

ABSTRACT: The buckling of short double-walled carbon nanotubes subjected to compression is investigated through molecular dynamics in the paper. The inner wall is discovered to have helically aligned buckling mode

while the outer wall is reported to have shell buckling mode with kinks. Such buckling modes are attributed to the interaction of the two walls via the van der Waals effect. In addition, a buckling strain higher than the buckling strains of two constituent inner and outer walls is found in the double-walled tube within a certain size range. The causes for such a phenomenon are analyzed and discussed.

A.R. Ranjbartoreh, A. Ghorbanpour and B. Soltani (Department of Mechanical Engineering, University of Kashan, Ghotb Ravandi Avenue, Kashan, 87317-51167, Iran), "Double-walled carbon nanotube with surrounding elastic medium under axial pressure", *Physica E: Low-dimensional Systems and Nanostructures*, Vol. 39, No. 2, September 2007, pp. 230-239, doi:10.1016/j.physe.2007.04.010

ABSTRACT: In this paper, the buckling behavior and critical axial pressure of double-walled carbon nanotubes (DWCNTs) with surrounding elastic medium are investigated. A double-shell (circular cylindrical shell) model is presented and the effects of surrounding elastic medium on the outer tube and the van der Waals forces between two adjacent tubes are taken into account. The analysis and the numerical solution method are based on the classical theory of plates and shells and the Galerkin method. Equations are derived for the critical axial forces and pressures of DWCNTs; the critical axial forces and pressures are calculated for different axial half sine wavenumbers and circumferential sine wavenumbers and compared with those for single-walled carbon nanotubes (SWCNTs). Results indicate that the critical axial force of a DWCNT is higher than that of an SWCNT, but the critical axial pressure of a DWCNT is lower than the critical axial pressure of a SWCNT. Although the critical axial force of a DWCNT decreases as the axial half sine wavenumbers increase, it rises as the circumferential sine wavenumbers increase.

A. Ghorbanpour Arani, R. Rahmani and A. Arefmanesh (Department of Mechanical Engineering, Faculty of Engineering, University of Kashan, Kashan, I.R., Iran), "Elastic buckling analysis of single-walled carbon nanotube under combined loading by using the ANSYS software", *Physica E: Low-dimensional Systems and Nanostructures*, Vol. 40, No. 7, May 2008, pp. 2390-2395, Special Issue: Proceedings of the E-MRS 2007 Symposia L and M: Electron Transport in Low-Dimensional Carbon Structures and Science and Technology of Nanotubes and Nanowires, doi:10.1016/j.physe.2007.11.011

ABSTRACT: This paper studies the pure axially compressed buckling and combined loading effects of a cylindrical shell and an individual single-walled carbon nanotube (SWCNT). The results of finite element (FE) simulations of SWCNT using the ANSYS software are presented, and are compared with the classical (local) and continuum (nonlocal) mechanical theories. Critical axial stress and deflections are calculated for all the cases. Two types of buckling are considered in this study, namely, the shell buckling which depends on the radius-to-thickness ratio, and the column buckling which is controlled by the length-to-diameter ratio.

Ghorbanpour Arani A., Rahmani R., Arefmanesh A., Golabi S., "Buckling analysis of multi-walled carbon nanotubes under combined loading considering the effect of small length scale", *Journal of Mechanical Science and Technology*, Vol. 22, No. 3, 2008, pp. 429-439, doi: 10.1007/s12206-007-1045-2

ABSTRACT: The torsional and axially compressed buckling of an individual embedded multi-walled carbon nanotube (MWNTs) subjected to an internal and/or external radial pressure was investigated in this study. The emphasis is placed on new physical phenomena which are due to both the small length scale and the surrounding elastic medium. Multiwall carbon nanotubes which are considered in this study are classified into three categories based on the radius to thickness ratio, namely, thin, thick, and almost solid. Explicit formulas are derived for the van der Waals (vdW) interaction between any two layers of an MWNT based on the continuum cylindrical shell model. In most of the previous studies, the vdW interaction between two adjacent layers was considered only and the vdW interaction among other layers was neglected. Moreover, in these works, the vdW interaction coefficient was treated as a constant that was independent of the radii of the tubes.

However, in the present model the vdW interaction coefficients are considered to be dependent on the change of interlayer spacing and the radii of the tubes. The effect of the small length scale is also considered in the present formulation. The results show that there is a unique buckling mode (m,n) corresponding to the critical shear stress. This result is obviously different from what is expected for the pure axially compressed buckling of an individual multi-walled carbon nanotube.

A. Ghorbanpour Arani, M. Shokravi, M. Mohammadimehr (Department of Mechanical Engineering, University of Kashan, Ravand, Kashan, Iran, email: a_ghorbanpour@yahoo.com (A. Ghorbanpour Arani).), "Buckling Analysis of a Double-Walled Carbon Nanotube Embedded in an Elastic Medium Using the Energy Method", *Archive of SID, Journal of Solid Mechanics* Vol. 1, No. 4 (2009) pp. 289-299

ABSTRACT: The axially compressed buckling of a double-walled carbon nanotube surrounded by an elastic medium using the energy and the Rayleigh-Ritz methods is investigated in this paper. In this research, based on the elastic shell models at nano scale, the effects of the van der Waals forces between the inner and the outer tubes, the small scale and the surrounding elastic medium on the critical buckling load are considered. Normal stresses at the outer tube medium interface are also included in the current analysis. An expression is derived relating the external pressure to the buckling mode number, from which the critical pressure can be obtained. It is seen from the results that the critical pressure is dependent on the outer radius to thickness ratio, the material parameters of the surrounding elastic medium such as Young's modulus and Poisson's ratio. Moreover, it is shown that the critical pressure descend very quickly with increasing the half axial wave numbers.

M. Mohammadimehr, A. R. Saidi, A. Ghorbanpour Arani, A. Arefmanesh and Q. Han, "Torsional buckling of a DWCNT embedded on winkler and pasternak foundations using nonlocal theory", *Journal of Mechanical Science and Technology*, Vol. 24, No. 6, 2010, pp. 1289-1299, doi: 10.1007/s12206-010-0331-6

ABSTRACT: The small-scale effect on the torsional buckling of a double-walled carbon nanotube (DWCNT) embedded on Winkler and Pasternak foundations is investigated in this study using the theory of nonlocal elasticity. The effects of the surrounding elastic medium, such as the spring constant of the Winkler type and the shear constant of the Pasternak type, as well as the van der Waals (vdW) forces between the inner and the outer nanotubes are taken into account. Finally, based on the theory of nonlocal elasticity and by employing the continuum models, an elastic double-shell model is presented for the nonlocal torsional buckling load of a DWCNT. It is seen from the results that the shear constant of the Pasternak type increases the nonlocal critical torsional buckling load, while the difference between the presence and the absence of the shear constant of the Pasternak type becomes large. It is shown that the nonlocal critical buckling load is lower than the local critical buckling load. Moreover, a simplified analysis is carried out to estimate the nonlocal critical torque for the torsional buckling of a DWCNT.

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"Thermal buckling analysis of double-walled carbon nanotubes considering the small-scale length effect", *Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science*, January 2011, vol. 225, no. 1, pp. 248-256, doi: 10.1177/09544062JMES1975

ABSTRACT: In this article, the buckling analysis of a double-walled carbon nanotube (DWCNT) subjected to a uniform internal pressure in a thermal field is investigated. The effects of the temperature change, the surrounding elastic medium based on the Winkler model, and the van der Waals forces between the inner and the outer tubes are considered using the continuum cylindrical shell model. The small-length scale effect is also included in the present formulation. The results show that there is a unique buckling mode corresponding to

each critical buckling load. Moreover, it is shown that the non-local critical buckling load is lower than the local critical buckling load. It is concluded that, at low temperatures, the critical buckling load for the infinitesimal buckling of a DWCNT increases as the magnitude of temperature change increases whereas at high temperatures, the critical buckling load decreases with the increasing of the temperature.

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“Postbuckling Equilibrium Path of a Long Thin-Walled Cylindrical Shell (Single-Walled Carbon Nanotube) Under Axial Compression Using Energy Method”, Archive of SID, IJE Transactions A: Basics, Vol. 24, No. 1, January 2011, pp. 79-86

ABSTRACT: In this paper, an elastic shell model is presented for postbuckling prediction of a long thin-walled cylindrical shell under axial compression. The Ritz method is applied to solve the governing equilibrium equation of a cylindrical shell model based on the von-Karman type nonlinear differential equations. The postbuckling equilibrium path is obtained using the energy method for a long thin-walled cylindrical shell. Furthermore, the postbuckling relationship between the axial stress and end-shortening is investigated with different geometric parameters. Also, this theory is used for postbuckling analysis of a single-walled carbon nanotube without considering the small scale effects. Numerical results reveal that the single-walled carbon nanotube under axial compression has an unstable postbuckling behavior.

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“Critical Strain of Carbon Nanotubes: An Atomic-Scale Finite Element Study”, J. Appl. Mech., Vol. 74, No. 2, March 2007, pp. 347-351, doi:10.1115/1.2198548

ABSTRACT: This paper employs the atomic-scale finite element method (AFEM) to study critical strain of axial buckling for carbon nanotubes (CNTs). Brenner et al. “second-generation” empirical potential is used to model covalent bonds among atoms. The computed energy curve and critical strain for (8, 0) single-walled CNT (SWNT) agree well with molecular dynamics simulations. Both local and global buckling are achieved, two corresponding buckling zones are obtained, and the global buckling behavior of SWNT with a larger aspect ratio approaches gradually to that of a column described by Euler's formula. For double-walled CNTs with smaller ratio of length to outer diameter, the local buckling behavior can be explained by conventional shell theory very well. AFEM is an efficient way to study buckling of CNTs.

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“Nonlocal shell model for elastic wave propagation in single- and double-walled carbon nanotubes”, Journal of

the Mechanics and Physics of Solids, Vol. 56, No. 12, December 2008, pp. 3475-3485,
doi:10.1016/j.jmps.2008.08.010

ABSTRACT: This paper investigates the transverse and torsional wave in single- and double-walled carbon nanotubes (SWCNTs and DWCNTs), focusing on the effect of carbon nanotube microstructure on wave dispersion. The SWCNTs and DWCNTs are modeled as nonlocal single and double elastic cylindrical shells. Molecular dynamics (MD) simulations indicate that the wave dispersion predicted by the nonlocal elastic cylindrical shell theory shows good agreement with that of the MD simulations in a wide frequency range up to the terahertz region. The nonlocal elastic shell theory provides a better prediction of the dispersion relationships than the classical shell theory when the wavenumber is large enough for the carbon nanotube microstructure to have a significant influence on the wave dispersion. The nonlocal shell models are required when the wavelengths are approximately less than 2.36×10^{-9} and 0.95×10^{-9} m for transverse wave in armchair (15,15) SWCNT and torsional wave in armchair (10,10) SWCNT, respectively. Moreover, an MD-based estimation of the scale coefficient e_0 for the nonlocal elastic cylindrical shell model is suggested. Due to the small-scale effects of SWCNTs and the interlayer van der Waals interaction of DWCNTs, the phase difference of the transverse wave in the inner and outer tube can be observed in MD simulations in wave propagation at high frequency. However, the van der Waals interaction has little effect on the phase difference of transverse wave.

Q. Wang (Department of Mechanical and Manufacturing Engineering, University of Manitoba, Winnipeg, Manitoba, Canada R3T 5V6), "Compressive buckling of carbon nanotubes containing polyethylene molecules", Carbon, Vol. 49, No. 2, February 2011, pp. 729-732, doi:10.1016/j.carbon.2010.10.023

ABSTRACT: The instability of a carbon nanotube containing a polyethylene molecule subjected to compression is investigated using molecular dynamics. A decrease up to 35% in the buckling strain of the (6,6) and (10,10) carbon nanotube/polymer structures due to the attractive van der Waals interaction between the tube wall and the polymer molecule is reported. In particular, the decrease in the buckling strain of the (6,6) carbon nanotube/polymer structure is attributed to the initiation of two flattenings on the tube wall. Simulations show that the buckling strain of the structure is insensitive to the number of units of the polymer molecule.

Q. Wang (Department of Mechanical and Manufacturing Engineering, University of Manitoba, Winnipeg, Manitoba, Canada R3T 5V6), "Buckling of carbon nanotubes wrapped by polyethylene molecules", Physics Letters A, Vol. 375, No. 3, January 2011, pp. 624-627, doi:10.1016/j.physleta.2010.12.005

ABSTRACT: The discovery of a buckling instability of a single-walled carbon nanotube wrapped by a polyethylene molecule subjected to compression is reported through molecular mechanics simulations. A decrease up to 44% in the buckling strain of the nano-structure owing to the van der Waals interaction between the two molecules is uncovered. A continuum model is developed to calculate both the interaction between the tube and the polymer and the decreased buckling strain of the structure by fitting the molecular mechanics results.

A.N. Guz (S.P. Timoshenko Institute of Mechanics, National Academy of Sciences of Ukraine, Kiev), "Three-dimensional theory of stability of a carbon nanotube in a matrix", International Applied Mechanics, Vol. 42, No.1, 2006, pp. 19-31, doi: 10.1007/s10778-006-0055-6

ABSTRACT: The three-dimensional theory of stability of a carbon nanotube (CNT) in a polymer matrix is presented. The results are obtained on the basis of the three-dimensional linearized theory of stability of deformable bodies. Flexural and helical (torsional) buckling modes are considered. It is proved that the helical (torsional) buckling modes occur in a single CNT (the interaction of neighboring CNTs is neglected) and do not occur in nanocomposites (the interaction of neighboring CNTs is taken into account).

Chunyu Li and Tsu-Wei Chou (Center for Composite Materials, Department of Mechanical Engineering, University of Delaware, 126 Spencer Laboratory, Newark, DE 19716-3140, USA), “Modeling of elastic buckling of carbon nanotubes by molecular structural mechanics approach”, *Mechanics of Materials*, Vol. 36, No. 11, November 2004, pp. 1047-1055, doi:10.1016/j.mechmat.2003.08.009

ABSTRACT: This paper reports the elastic buckling behavior of carbon nanotubes. Both axial compression and bending loading conditions are considered. The modeling work employs the molecular structural mechanics approach for individual nanotubes and considers van der Waals interaction in multi-walled nanotubes. The effects of nanotube diameter, aspect ratio, and tube chirality on the buckling force are investigated.

Computational results indicate that the buckling force in axial compression is higher than that in bending, and the buckling forces for both compression and bending decrease with the increase in nanotube aspect ratio. The trends of variation of buckling forces with nanotube diameter are similar for single-walled and double-walled carbon nanotubes. Compared to a single-walled nanotube of the same inner diameter, the double-walled carbon nanotube shows a higher axial compressive buckling load, which mainly results from the increase of cross-sectional area, but no enhancement in bending load-bearing capacity. The buckling forces of nanotubes predicted by the continuum beam or column models are significantly different from those predicted by the atomistic model.

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“Buckling analysis of multi-walled carbon nanotubes: a continuum model accounting for van der Waals interaction”, *Journal of the Mechanics and Physics of Solids*, Vol. 53, No. 2, February 2005, pp. 303-326, doi:10.1016/j.jmps.2004.08.003

ABSTRACT: Explicit formulas are derived for the van der Waals (vdW) interaction between any two layers of a multi-walled carbon nanotube (CNT). Based on the derived formulas, an efficient algorithm is established for the buckling analysis of multi-walled CNTs, in which individual tubes are modeled as a continuum cylindrical shell. The explicit expressions are also derived for the buckling of double-walled CNTs. In previous studies by Ru (*J. Appl. Phys.* 87 (2000b) 7227) and Wang et al. (*Int. J. Solids Struct.* 40 (2003) 3893), only the vdW interaction between adjacent two layers was considered and the vdW interaction between the other two layers was neglected. The vdW interaction coefficient was treated as a constant that was not dependent on the radii of the tubes. However, the formulas derived herein reveal that the vdW interaction coefficients are dependent on the change of interlayer spacing and the radii of the tubes. With the increase of radii, the coefficients approach constants, and the constants between two adjacent layers are about 10% higher than those reported by Wang et al. (*Int. J. Solids Struct.* 40 (2003) 3893). In addition, the numerical results show that the vdW interaction will lead to a higher critical buckling load in multi-walled CNTs. The effect of the tube radius on the critical buckling load of a multi-walled CNT is also examined.

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“Buckling and Postbuckling Analysis of Multi-Walled Carbon Nanotubes Based on the Continuum Shell Model”, *International Journal of Structural Stability and Dynamics* Vol. 7, No. 4 (2007) pp. 629–645

ABSTRACT: Buckling and postbuckling behaviors of multi-walled carbon nanotubes (MWCNTs) under a compressive force are studied. MWCNTs are modeled by Donnell’s shallow shell nonlinear theory with the allowance of van der Waals (vdW) interaction between the walls. It is shown herein that the buckling load decreases while the buckling strain increases as the innermost radius of MWCNT increases. For the postbuckling behavior, the shortening-load curves show an initial steep gradient that gradually level up when the radius of the innermost tube changes from a small value to a large value. However, the deflection-load curves are almost level for various radii of MWCNTs. In addition, the analytical results showed that the shortening-load curves are almost linear but the deflection-load curves are nonlinear and the stability of MWCNTs can be enhanced by adding tubes.

Liew, K. M., Wang, J. B., He, X. Q. and Zhang, H. W. (Department of Building and Construction, City University of Hong Kong, Kowloon, Hong Kong), “Buckling analysis of abnormal multiwalled carbon nanotubes”, *Journal of Applied Physics*, Vol. 102, No. 10, September 2007, pp. 053511-053511-6, doi: 10.1063/1.2777893

ABSTRACT: Abnormal multiwalled carbon nanotubes (MWNTs) with an interlayer distance of less than 0.34 nm are proposed and optimized based on molecular dynamics simulation, in which the second-generation Tersoff-Brenner potential and Lennard-Jones (12-6) potential are used to characterize the intratube interatomic interaction and the intertube van der Waals (vdW) interaction, respectively. Then, a multishell continuum model that is combined with a refined vdW force model is used to carry out the buckling analysis of abnormal MWNTs (including two-, four-, and six-walled MWNTs) and to investigate the effect of the vdW interaction of abnormal MWNTs. The numerical results show that the effect of the vdW interaction is more significant for abnormal MWNTs than for normal MWNTs and that the vdW interaction of abnormal MWNTs cannot be neglected. The critical buckling strains of abnormal MWNTs are greatly enhanced compared with those of normal MWNTs, which suggests that abnormal MWNTs may be excellent candidates as enforced fibers of nanocomposites.

F. Khademolhosseini, R.K.N.D. Rajapakse, A. Nojeh, “Torsional buckling of carbon nanotubes based on nonlocal elasticity shell models”, *Computational Materials Science*, Elsevier, Vol. 48, pp.736-742 (2010)
Abstract: This paper investigates size-effects in the torsional response of single walled carbon nanotubes (SWCNTs) by developing a modified nonlocal continuum shell model. The purpose is to facilitate the design of devices based on SWCNT torsion by providing a simple, accurate and efficient continuum model that can predict the corresponding buckling loads. To this end, Eringen’s equations of nonlocal elasticity are incorporated into the classical models for torsion of cylindrical shells given by Timoshenko and Donnell. In contrast to the classical models, the nonlocal model developed here predicts non-dimensional buckling torques that depend on the values of certain geometric parameters of the CNT, allowing for the inclusion of size-effects. Molecular dynamics simulations of torsional buckling are also performed and the results of which are compared with the classical and nonlocal models and used to extract consistent values of shell thickness and the nonlocal elasticity constant (ϵ_0). A thickness of 0.85 Å and nonlocal constant values of approximately 0.8 and 0.6 for armchair and zigzag nanotubes respectively are recommended for torsional analysis of SWCNTs using nonlocal shell models. The size-dependent nonlocal models together with molecular dynamics simulations show that classical shell models overestimate the critical buckling torque of SWCNTs and are not suitable for modeling of SWCNTs with diameters smaller than 1.5 nm.

A. Montazeri and R. Naghdabadi, Institute for Nano Science and Technology, Sharif University of Technology, 14588-89694 Tehran, Iran, “Investigating the Effect of Carbon Nanotube Defects on the Column and Shell Buckling of Carbon Nanotube-Polymer Composites Using Multiscale Modeling”,

doi: 10.1615/IntJMultCompEng.v7.i5.50

ABSTRACT: Carbon nanotube (CNT)-reinforced polymer composites have attracted great attention due to their exceptionally high strength. Their high strength can be affected by the presence of defects in the nanotubes used as reinforcements in practical nanocomposites. In this article, a new three-phase molecular structural mechanics/finite element (MSM/FE) multiscale model is used to study the effect of CNT vacancy defects on the stability of single-wall (SW) CNT-polymer composites. The nanotube is modeled at the atomistic scale using MSM, whereas the interphase layer and polymer matrix are analyzed by the FE method. The nanotube and polymer matrix are assumed to be bonded by van der Waals interactions based on the Lennard-Jones potential. Here, two of the most commonly used buckling regimes of CNTs, called column and shell buckling, are considered. To study the stability of the nanocomposites, the buckling onset strain is calculated for perfect and defected CNTs in the polymer nanocomposites. The results reveal that the presence of vacancy defects causes a decrease in the axial buckling strain of SWCNT-polymer composites. Meanwhile, this decrease is much more noticeable in the case of the column buckling mode. Also, it is shown that decreasing the CNT diameter causes a reduction in the onset buckling strain of defected nanocomposites. Finally, the role of the interphase layer on the stability behavior of these nanocomposites is discussed. It is concluded that the existence of a more compact layer than the polymer chains coated on the nanotube can enhance drastically the buckling behavior of these nanocomposites (about 35%).

I-Ling Chang and Bing-Chen Chiang (Department of Mechanical Engineering, National Chung Cheng University, Chia-Yi 621, Taiwan), “Mechanical buckling of single-walled carbon nanotubes: Atomistic simulations”, *Journal of Applied Physics*, Vol. 106, No. 11, December 2009, pp. 114313-114313-5,

doi: 10.1063/1.3260239

ABSTRACT: Various geometric sizes and helical types (i.e., armchair, zigzag, and chiral) of single-walled carbon nanotubes (CNTs) are considered in molecular dynamics simulations in order to systematically examine the length-to-radius ratio and chirality effects on the buckling mechanism. The buckling strain is getting smaller as the CNT becomes slender for most nanotubes, which implies that the slender nanotubes have lower buckling resistance regardless of the radius of the CNTs. The applicability of the continuum buckling theory, which has been well developed for thin tubes, on predicting the buckling strain of the CNT is also examined. In general, the corresponding buckling strain and buckling type predicted by the continuum buckling theory could agree reasonably well with simulation results except at the transition region due to the competition of two buckling mechanisms.

Guoxin Cao and Xi Chen (Columbia Nanomechanics Research Center, Department of Civil Engineering and Engineering Mechanics, Columbia University, New York, NY 10027-6699, USA,

email: xichen@civil.columbia.edu), “The effect of the displacement increment on the axial compressive buckling behaviours of single-walled carbon nanotubes”, *Nanotechnology* Vol. 17, No. 15, 2006, p.3844,

doi: 10.1088/0957-4484/17/15/040

ABSTRACT: We carry out systematic molecular mechanics (MM) analyses to study the effect of the displacement increment on the critical buckling strain of single-walled carbon nanotubes (SWCNTs) under axial compression. The SWCNT geometric parameters, such as the tube length, diameter, and chirality, are varied in the numerical studies. The results show that the critical buckling strain of the SWCNTs deduced from the atomistic analyses is highly sensitive to the displacement increment used in the numerical simulation, and such an effect is more obvious for tubes with smaller diameters. Therefore, a reasonable compressive

displacement increment should be selected in the atomistic simulations in order to obtain the intrinsic values of the critical buckling strain, which is suggested in this paper. The studies in this paper may be used to explain the contradicting results of the critical compressive buckling strains computed by other MM analyses in the literature.

Guoxin Cao and Xi Chen (Nanomechanics Research Center, Department of Civil Engineering and Engineering Mechanics, Columbia University, New York, New York 10027, USA), “Buckling of single-walled carbon nanotubes upon bending: Molecular dynamics simulations and finite element method”, *Phys. Rev. B* Vol. 73, 2006, 155435 [10 pages], doi: 10.1103/PhysRevB.73.155435

ABSTRACT: The bending buckling behaviors of single-walled carbon nanotubes (SWCNTs) are systematically investigated by using both molecular dynamics (MD) simulation and finite element method (FEM), to analyze the relationships between critical bending buckling curvature, critical buckling strain and nanotube geometry parameters (e.g., tube diameter, length and chirality). The postbuckling shape of SWCNT and the effect of loading boundary conditions are also discussed. The comparison between MD and FEM simulations shows that the continuum shell model provides some useful insights into the bending buckling mechanisms, yet it cannot quantitatively reproduce the bending buckling behavior of SWCNTs, since the continuum model does not account for the geometrical imperfections in the atomic system that are critical to the onset of buckling. Improvements of continuum models are suggested based on the findings.

Guoxin Cao and Xi Chen (Columbia Nanomechanics Research Center, Department of Civil Engineering and Engineering Mechanics, Columbia University, New York, New York 10027-6699, USA), “Buckling behavior of single-walled carbon nanotubes and a targeted molecular mechanics approach”, *Phys. Rev. B* 74, 165422 (2006) [10 pages], doi: 10.1103/PhysRevB.74.165422

ABSTRACT: During the general (conventional) molecular mechanics (GMM) simulation of the buckling of single-walled carbon nanotubes (SWCNTs), the load is displacement controlled and the calculated critical buckling strain is very sensitive to the specific displacement increment and convergence threshold chosen in molecular dynamics (MD) simulations, which may have led to the contradictory and diverged results in the previous studies. In this paper, a targeted-molecular mechanics (TMM) simulation method is proposed to study the buckling behavior of SWCNTs under axial compression, bending, and torsion. Comparing with the GMM method, the TMM technique is independent of the displacement increment and thus the solution is converged. The critical buckling strain computed from the TMM is higher than that from the GMM under axial compression and torsion, and the TMM results are similar to the GMM results upon bending. The TMM result approaches to the intrinsic critical buckling strain of a perfect tube; in addition, the TMM significantly reduces the computational cost and thus may be more efficient to study larger systems with atomistic simulations.

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“Application of Nonlocal Elasticity Shell Model for Axial Buckling of Single-Walled Carbon Nanotubes”, *MEMS: From Micro Devices to Wireless Systems*, Vol. 7, Special Issue, October 2009, pp.88-100.

ABSTRACT:

Recently, nano devices have been developed which use Carbon Nanotubes (CNTs) as structural elements. To define the range of applicability of CNTs in such devices, it is important to investigate failure modes such as the axial buckling limit. Classical continuum models are inaccurate as they are unable to account for the size-effects in such devices. In this work, a modified nonlocal continuum shell model for the axial buckling of CNTs is proposed and compared with a nonlocal model for torsional buckling. This is done through modifying classical

continuum models by incorporating basic concepts from nonlocal elasticity. Furthermore, molecular dynamics (MD) simulations are performed on a range of nanotubes with different diameters. Compared to classical models, the modified nonlocal models provide a much better fit to MD simulation results. Using MD simulation results for axial buckling, values of the nonlocal constant and shell thickness are calculated.

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“Nanomechanics of single and multiwalled carbon nanotubes”, *Phys. Rev. B* 69, 115429 (2004) [8 pages], doi: 10.1103/PhysRevB.69.115429

ABSTRACT: Buckling behavior of single-walled and multiwalled carbon nanotubes is studied under axial compression in this work. Brenner's “second generation” empirical potential is used to describe the many-body short-range interatomic interactions for single-walled carbon nanotubes, while the Lennard Jones model for the van der Waals potential is added for multiwalled carbon nanotubes. Single-, two-, three-, and four-walled nanotubes are considered in the simulations in order to examine the effects of the number of layers on the structural properties of the multiwalled nanotubes. Results indicate that there exists an optimum diameter for single-walled nanotubes at which the buckling load reaches its maximum value. The buckling load increases rapidly with the increase of the diameter up to the optimum diameter. A further increment beyond this diameter results in a slow decline in buckling load until a steady value is reached. The effects of layers on the buckling load of multiwalled nanotubes are also examined.

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“Modeling of the mechanical instability of carbon nanotubes”, *Carbon*, Vol. 46, No. 2, February 2008, pp. 285-290, doi:10.1016/j.carbon.2007.11.022

ABSTRACT: A hybrid continuum mechanics and molecular mechanics model is developed to predict the compressive buckling strain and load for the inelastic buckling of armchair and zigzag carbon nanotubes. The effectiveness of the hybrid model is demonstrated by comparisons of buckling results from the model, molecular dynamics simulations, and continuum models by other work.

Yuzhou Sun and K.M. Liew (Department of Building and Construction, City University of Hong Kong, Kowloon, Hong Kong), “The buckling of single-walled carbon nanotubes upon bending: The higher order gradient continuum and mesh-free method”, *Computer Methods in Applied Mechanics and Engineering*, Vol. 197, Nos. 33-40, 1 June 2008, pp. 3001-3013, doi:10.1016/j.cma.2008.02.003

ABSTRACT: The bending buckling of single-walled carbon nanotubes (SWCNTs) is studied in the theoretical scheme of the higher order gradient continuum. The deformation of the underlying lattice vectors is approximated with an extended Cauchy–Born rule in which the effect of the second order deformation gradient is considered, and the continuum constitutive responses are determined by minimizing the energy of the representative cell. A mesh-free method is developed to implement the numerical modeling of SWCNTs, and their bending buckling behavior is numerically simulated with the developed method. The results are compared

with those obtained with a full atomistic simulation, and it is revealed that the developed mesh-free method can accurately exhibit the bending deformation of SWCNTs. Different types of carbon nanotubes (CNTs) are studied, and the buckling mechanism is investigated.

Reshef Tenne and Alex K. Zettl, "Nanotubes from Inorganic Materials", Carbon Nanotubes, Topics in Applied Physics, 2001, Vol. 80, 2001, pp. 81-112, doi: 10.1007/3-540-39947-X_5

ABSTRACT: The inorganic analogs of carbon fullerenes and nanotubes, like MoS₂ and BN, are reviewed. It is argued that nanoparticles of 2D layered compounds are inherently unstable in the planar configuration and prefer to form closed cage structures. The progress in the synthesis of these nanomaterials, and, in particular, the large-scale synthesis of BN, WS₂ and V₂O₅ nanotubes, are described. Some of the electronic, optical and mechanical properties of these nanostructures are reviewed. The red-shift of the energy gap with shrinking nanotube diameter is discussed as well as the suggestion that zigzag nanotubes exhibit a direct gap rather than an indirect gap, as is prevalent in many of the bulk 2D materials. Some potential applications of these nanomaterials are presented as well, most importantly the superior tribological properties of WS₂ and MoS₂ nested fullerene-like structures (onions).

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"Buckling instabilities in GaN nanotubes under uniaxial compression", Institute Of Physics Publishing: Nanotechnology 16 (2005) 2203–2208.

ABSTRACT: We report experimental observations of shell buckling instabilities in free-standing, vertically aligned GaN nanotubes subjected to uniaxial compression. Highly uniform arrays of the GaN nanotubes standing on a GaN template were fabricated and subjected to uniaxial compression using a nanoindenter. The buckling load was found to be of the order of 150 μ N for the GaN nanotubes with an outer radius of 40 nm, an inner radius of 20 nm, and heights of 500 and 300 nm. Good agreement was found between the experimental observations, the stress–strain relation equation study findings and the predictions from the cylindrical shell buckling theory.

X. Wang, H.K. Yang and K. Dong (Department of Engineering Mechanics, School of Naval Architecture, Ocean and Civil Engineering, Shanghai Jiaotong University, Shanghai 200240, PR China), "Torsional buckling of multi-walled carbon nanotubes", Materials Science and Engineering: A, Vol. 404, Nos. 1-2, September 2005, pp. 314-322, doi:10.1016/j.msea.2005.05.071

ABSTRACT: This paper investigates torsional buckling of an individual multi-walled carbon nanotubes. The multiple shell model is adopted and the effect of van der Waals forces between adjacent nanotubes is taken into account. According to the ratio of radius-to-thickness, multi-walled carbon nanotubes discussed here are classified into three cases: thin, thick, and nearly solid. The critical shear stress and the torsional buckling mode are calculated for various radius-to-thickness ratios. Results carried out show that the buckling mode (m, n) corresponding the critical shear stress is sole, which is obviously different from the axially compressed buckling of an individual multi-walled carbon nanotubes. The investigation on torsional buckling of multi-walled carbon nanotubes in this paper may be used as a useful reference for the designs of nano-oscillators, nano-drive devices and actuators in which multi-walled carbon nanotubes act as basic elements.

Y.J. Lu and X. Wang (Department of Engineering Mechanics, School of Naval Architecture, Ocean and Civil Engineering, Shanghai Jiaotong University, Shanghai 200240, People's Republic of China, email: xwang@sjtu.edu.cn), "Combined torsional buckling of multi-walled carbon nanotubes", J. Phys. D: Appl. Phys. Vol. 39, 2006, p. 3380 doi: 10.1088/0022-3727/39/15/024

ABSTRACT: This paper reports the results of an investigation on combined torsional buckling of an individual multi-walled carbon nanotube (MWNT) under combined torque and axial loading. Here, a multiple shell model is adopted and the effect of van der Waals forces between two adjacent tubes is taken into account. According to the ratio of radius to thickness, MWNTs discussed in this paper are classified into three types: thin, thick and nearly solid. The critical shear stress and the combined buckling mode are calculated for three types of MWNTs under combined torque and axial loading. Results carried out show that the buckling mode (m, n) corresponding to the critical shear stress is unique, which is obviously different from the purely axial compression buckling of an individual MWNT. Numerical results also show that the critical shear stresses and the corresponding buckling modes of MWNTs under combined torque and axial loading are dependent on the axial loading form and the types of MWNTs. The new features and meaningful numerical results in the present work on combined buckling of MWNTs under combined torque and axial loading may be used as a useful reference for the designs of nano-drive devices and rotational actuators in which MWNTs act as basic elements.

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"Buckling of embedded multi-walled carbon nanotubes under combined torsion and axial loading", International Journal of Solids and Structures, Vol. 44, No. 1, January 2007, pp. 336-351, doi:10.1016/j.ijsolstr.2006.04.031

ABSTRACT: This paper describes an investigation into elastic buckling of an embedded multi-walled carbon nanotube under combined torsion and axial loading, which takes account of the radial constraint from the surrounding elastic medium and van der Waals force between two adjacent tube walls. Depending on the ratio of radius to thickness, the multi-walled carbon nanotubes discussed here are classified as thin, thick, and nearly solid. Critical buckling load with the corresponding mode is obtained for multi-walled carbon nanotubes under combined torsion and axial loading, with various values of the radius to thickness ratio and surrounded with different elastic media. The study indicates that the buckling mode (m, n) of an embedded multi-walled carbon nanotube under combined torsion and axial loading is unique and it is different from that with axial compression only. New features for the buckling of an embedded multi-walled carbon nanotube under combined torsion and axial loading and the meaningful numerical results are useful in the design of nanodrive device, nanotorsional oscillator and rotational actuators, where multi-walled carbon nanotubes act as basic elements.

H.K. Yang and X. Wang (Department of Engineering Mechanics, School of Naval Architecture, Ocean and Civil Engineering, Shanghai Jiaotong University, Shanghai 200240, People's Republic of China), "Torsional buckling of multi-wall carbon nanotubes embedded in an elastic medium", Composite Structures, Vol. 77, No.2, January 2007, pp. 182-192, doi:10.1016/j.compstruct.2005.06.013

ABSTRACT: This paper investigates torsional buckling of a multi-wall carbon nanotube embedded in an elastic medium. The effects of surrounding elastic medium and van der Waals forces from adjacent nanotubes are taken into account. Using continuum mechanics, an elastic laminated shell model is presented to study the torsional buckling of a multi-wall carbon nanotube embedded in an elastic medium. A laminated cylinder

composed of a multi-wall carbon nanotube and a surrounding elastic medium is used to describe the effect of elastic medium on the multi-wall carbon nanotubes. According to the ratio of radius-to-thickness, multi-wall carbon nanotubes discussed here are classified into three cases: thin, thick, and nearly solid. The critical shear stress and the torsional buckling mode are calculated for various radius-to-thickness ratios and elastic medium effects. Results carried out show that the buckling mode (m, n) corresponding the critical shear stress is sole, which is obviously different from the axially compressed buckling of multi-wall carbon nanotubes. The investigation on torsional buckling of multi-wall carbon nanotubes embedded in an elastic medium in this paper may be used as a useful reference for the designs of nano-oscillators and actuators in which multi-wall carbon nanotubes act as torsional springs.

X.Y. Wang and X. Wang (Department of Engineering Mechanics, School of Naval Architecture Ocean and Civil Engineering, Shanghai Jiaotong University Shanghai 200240, P.R. China, email: xwang@sjtu.edu.cn), "Torsional Buckling of Multi-walled Carbon Nanotubes Subjected to Torsional Loads", *Journal of Reinforced Plastics and Composites*, March 2007, vol. 26, no. 5, pp. 479-494, doi: 10.1177/0731684406072538

ABSTRACT: The torsional buckling of an individual multi-walled carbon nanotube under two different loading conditions is studied in this article. The multiple shell model is adopted and the effects of van der Waals forces between adjacent nanotubes are taken into account. An examination with an individual double-walled carbon nanotube shows that the effect of the change of interlayer spacing on the torsional buckling force can be neglected if only the innermost radius is larger than a certain value. Under this condition, single buckling equations are derived and explicit formulas for the critical torsional loads in terms of the buckling modes are obtained. It is found that the critical torsional load of a multi-walled carbon nanotube with torque exerted on the outermost tube is higher than that of the same multi-walled carbon nanotubes under the torques being proportionally applied to each individual layer of the multi-walled carbon nanotubes. For thin multi-walled carbon nanotubes with large radii, the critical torque linearly scales with its thickness, but the critical shear force (per unit length) of the multi-walled carbon nanotubes uniformly twisted along the cross section does not increase as its layer number (thickness) increases, which is due to the interlayer slips between adjacent nanotubes.

Hsao W. Yap, Roderic S. Lakes, and Robert W. Carpick (Department of Physics, Department of Engineering Physics, Materials Science Program, and Rheology Research Center, University of Wisconsin-Madison, Madison, Wisconsin 53706), "Mechanical Instabilities of Individual Multiwalled Carbon Nanotubes under Cyclic Axial Compression", *Nano Letters*, 2007, Vol. 7, No. 5, pp. 1149-1154, doi: 10.1021/nl062763b

ABSTRACT: Individual multiwalled carbon nanotubes with a range of aspect ratios are subjected to cyclic axial compression to large strains using atomic force microscopy. Distinct elastic buckling and postbuckling phenomena are observed reproducibly and are ascribed to Euler, asymmetric shell buckling (i.e., kinking), and symmetric shell buckling. These show agreement with continuum theories that range from approximate to remarkable. Shell buckling yields reproducible incremental negative stiffness in the initial postbuckled regime.

Irene Arias and Marino Arroyo (Dept. Applied Mathematics 3, LaCàN, Universitat Politècnica de Catalunya (UPC), Barcelona 08034, Spain), "Size-Dependent Nonlinear Elastic Scaling of Multiwalled Carbon Nanotubes", *Phys. Rev. Lett.*, Vol. 100, 085503 (2008) [4 pages], doi: 10.1103/PhysRevLett.100.085503

ABSTRACT: We characterize through large-scale simulations the nonlinear elastic response of multiwalled carbon nanotubes (MWCNTs) in torsion and bending. We identify a unified law consisting of two distinct power law regimes in the energy-deformation relation. This law encapsulates the complex mechanics of rippling and is described in terms of elastic constants, a critical length scale, and an anharmonic energy-deformation exponent. The mechanical response of MWCNTs is found to be strongly size dependent, in that the critical strain beyond which they behave nonlinearly scales as the inverse of their diameter. These predictions are consistent with available

experimental observations.

Richard Superfine, Michael Falvo, Russell M. Taylor, II and Sean Washburn (Department of Physics and Astronomy, North Carolina University at Chapel Hill), “Nanomanipulation: Buckling, Transport and Rolling at the Nanoscale”, Research Report, 2002

DTIC Accession Number: ADA466718, Handle / proxy Url : <http://handle.dtic.mil/100.2/ADA466718>

ABSTRACT: The study of novel materials produces many challenges in the areas of synthesis, modeling and characterization. For the latter, one would like to be able to determine mechanical, electrical and dynamical properties, and correlate them with structure. In the following chapter, we describe work performed at the University of North Carolina-Chapel Hill (UNC) in the development of microscopy instrument systems, including a natural interface for scanned probe microscopy we call the nanoManipulator. We describe the principle design features of the instrument system including the visual display of data, the haptic (force-feedback) control and display capabilities. Second, we describe the combination of microscopy and manipulation in a joint Scanning Electron Microscopy/Scanning Probe Microscopy system. These systems have been used for studies of nanotube mechanical dynamical and electrical properties,⁸ and for the study of biological macromolecular structures such as viruses, fibers (pili, fibrin, microtubules, etc.) and molecules (DNA). We describe examples of these studies drawn from our work on nanotubes and viruses.

L. J. Sudak (Department of Mechanical and Manufacturing Engineering, University of Calgary, Calgary, Alberta T2N-1N4, Canada), “Column buckling of multiwalled carbon nanotubes using nonlocal continuum mechanics”, J. Appl. Phys. 94, 7281 (2003); doi:10.1063/1.1625437 (7 pages),

ABSTRACT: A model, based on the theory of nonlocal continuum mechanics, on the column buckling of multiwalled carbon nanotubes is presented. The present analysis considers that each of the nested concentric tubes is an individual column and that the deflection of all the columns is coupled together through the van der Waals interactions between adjacent tubes. Based on this description, a condition is derived in terms of the parameters that describe the van der Waals forces and the small internal length scale effects. In particular, an explicit expression is derived for the critical axial strain of a double walled carbon nanotube which clearly demonstrates that small scale effects contribute significantly to the mechanical behavior of multiwalled carbon nanotubes and cannot be ignored.

C.Q. Ru (Department of Mechanical Engineering, University of Alberta, Edmonton, Alberta T6G 2G8, Canada), “Column buckling of multiwalled carbon nanotubes with interlayer radial displacements”, Phys. Rev. B, Vol. 62, pp.16962–16967 (2000), doi: 10.1103/PhysRevB.62.16962

ABSTRACT: An elastic model is presented for column buckling of a multiwalled carbon nanotube embedded within an elastic medium. The emphasis is placed on the role of interlayer radial displacements between adjacent nanotubes. In contrast to an existing model which treats the entire multiwalled nanotube as a single column, the present model treats each of the nested tubes as an individual column interacting with adjacent nanotubes through the intertube van der Waals forces. Based on this model, a condition is derived in terms of the parameters describing the van der Waals interaction, under which the effect of the noncoincidence of all deflected column axes is so small that it does not virtually affect the critical axial strain. In particular, this condition is met for carbon multiwalled nanotubes provided that the half-wavelength of the buckling mode is much larger than the outermost diameter. In this case, the critical axial strain can be predicted correctly by the existing single-column model. On the other hand, the existing model could overestimate the critical axial strain when the half-wavelength of the buckling mode is close to or smaller than the outermost radius.

C. Q. Ru (Department of Mechanical Engineering, University of Alberta, Edmonton, Alberta T6G 2G8, Canada), “Degraded axial buckling strain of multiwalled carbon nanotubes due to interlayer slips”, J. Appl. Phys. 89, 3426

(2001); doi:10.1063/1.1347956 (8 pages)

ABSTRACT: A multiple-shell model is presented for infinitesimal axially compressed buckling of a multiwalled carbon nanotube embedded within an elastic matrix. In contrast to an existing single-shell model which treats the entire multiwalled nanotube as a single layer elastic shell, the present model assumes that each of the nested concentric tubes is an individual elastic shell and the deflections of all shells are coupled through the van der Waals interaction between adjacent nanotubes. By examining a doublewalled carbon nanotube, it is found that the change in interlayer spacing has a negligible effect on the axial buckling strain provided that the innermost radius is at least a few nanometers. Under this condition, a single equation is derived which determines the deflection of the multiwalled carbon nanotube, and it is shown that infinitesimal axial buckling of a N-walled carbon nanotubes is equivalent to that of a single layer elastic shell whose bending stiffness is approximately N times the effective bending stiffness of a single walled carbon nanotube. As a result, the axial buckling strain of a N-walled carbon nanotube is about 5 N times lower than that predicted by the existing single-shell model. The degraded axial buckling strain is attributed to the interlayer slips between adjacent nanotubes, which represents an essential feature of mechanical behavior of multiwalled carbon nanotubes

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“Compressive Instability of Carbon Nanotubes”, Key Engineering Materials Vols. 353-358 (2007) pp. 2187-2190 online at <http://www.scientific.net> Online available since 2007/09/10

ABSTRACT: Abstract. Based on both molecular mechanics and computational structural mechanics, a three-dimensional (3D) equivalent beam element is developed to model a C-C covalent bond on carbon nanotubes (CNTs) whereas the van der Waals forces between atoms in the different walls of multi-walled CNTs are described using a rod element. The buckling characteristics of CNTs are conveniently analyzed by using the traditional finite element method (FEM) of a 3D beam and rod model, termed as molecular structural mechanics approach (MSMA). Moreover, to model the CNTs with large length or large diameter, the validity of Euler's beam buckling theory and a shell model with proper properties defined from the results of MSMA is investigated. The predicted results by this simple continuum mechanics approach agree well with the reported experimental data.

Devesh Kumar, Christian Heinrich, and Anthony M. Waas (Department of Aerospace Engineering, University of Michigan, Ann Arbor, MI 48109, USA), “Buckling analysis of carbon nanotubes modeled using nonlocal continuum theories”, J. Appl. Phys. 103, 073521 (2008); doi:10.1063/1.2901201 (8 pages)

ABSTRACT: In this paper, the buckling of carbon nanotubes, modeled as nonlocal one dimensional continua within the framework of Euler–Bernoulli beams, is considered. Both a stress gradient and a strain gradient approach are considered and a variational approach is adopted to obtain the variationally consistent boundary conditions. The dependence of the buckling load on the nonlocal parameter has been determined using the boundary conditions obtained from the variational analysis. Results indicate significant dependence of nonlocal parameter on buckling load for particular types of boundary conditions. These findings are important in mechanical design considerations of devices that use carbon nanotubes.

Hui-Shen Shen (School of Civil Engineering and Mechanics, Shanghai Jiao Tong University, 1954 Hua Shan Road, Shanghai 200030, People's Republic of China), “Postbuckling prediction of double-walled carbon nanotubes under hydrostatic pressure”, International Journal of Solids and Structures, Vol. 41, Nos. 9-10, May 2004, pp. 2643-2657, doi:10.1016/j.ijsolstr.2003.11.028

ABSTRACT: An elastic double-shell model is presented for the buckling and postbuckling of a double-walled carbon nanotube subjected to external hydrostatic pressure. The analysis is based on a continuum mechanics model in which each tube of a double-walled carbon nanotube is described as an individual elastic shell and the interlayer friction is negligible between the inner and outer tubes. The governing equations are based on higher order shear deformation shell theory with a von Kármán–Donnell-type of kinematic nonlinearity. The van der Waals interaction between the inner and outer nanotubes and the nonlinear prebuckling deformations of the shell are both taken into account. A boundary layer theory of shell buckling is extended to the case of double-walled carbon nanotubes under hydrostatic pressure. A singular perturbation technique is employed to determine the buckling loads and postbuckling equilibrium paths. Numerical results reveal that the single-walled carbon nanotube has a stable postbuckling path, whereas the double-walled carbon nanotube has an unstable postbuckling behavior due to the presence of van der Waals interaction forces.

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“Free transverse vibrations of double-walled carbon nanotubes using a theory of nonlocal elasticity”, *Phys. Rev. B* 71, 195404 (2005) [7 pages], doi: 10.1103/PhysRevB.71.195404

ABSTRACT: Based on theory of nonlocal elasticity, a nonlocal double-elastic beam model is developed for the free transverse vibrations of double-walled carbon nanotubes. The effect of small length scale is incorporated in the formulation. With this nonlocal double-elastic beam model, explicit expressions are derived for natural frequencies and associated amplitude ratios of the inner to the outer tubes for the case of simply supported double-walled carbon nanotubes. The effect of small length scale on the properties of vibrations is discussed. It is demonstrated that the natural frequencies and the associated amplitude ratios of the inner to the outer tubes are dependent upon the small length scale. The effect of small length scale is related to the vibrational mode and the aspect ratio.

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“Investigation of buckling of double-walled carbon nanotubes embedded in an elastic medium using the energy method”, *International Journal of Mechanical Sciences*, Vol. 48, No. 1, January 2006, pp. 53-61, doi:10.1016/j.ijmecsci.2005.09.010

ABSTRACT: Elastic buckling of a long double-walled carbon nanotube embedded in an elastic medium and subjected to a far-field hydrostatic pressure is analyzed using the energy method. The study is on the basis of elastic-shell models at nano-scale, and the effect of van der Waals forces on the buckling is considered. The double-walled carbon nanotube is assumed to be thin and the tube is taken to be perfectly bonded to the surrounding medium. Both normal and shear stresses at the outer tube-medium interface are included. The difference between the Poisson's ratio of the tube and that of the elastic medium is taken into account. An expression is derived relating the external pressure to the buckling mode number, from which the critical pressure can be obtained. As a result, the critical pressure is dependent on the inner radius-to-thickness ratio, the material parameters of the elastic medium, and the van der Waals force.

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“Effect of small length scale on elastic buckling of multi-walled carbon nanotubes under radial pressure”, *Physics Letters A*, Vol. 349, No. 5, January 2006, pp. 370-376, doi:10.1016/j.physleta.2005.09.036

ABSTRACT: A nonlocal multiple-shell model is developed for the elastic buckling of multi-walled carbon nanotubes under uniform external radial pressure on the basis of theory of nonlocal elasticity. The effect of small length scale is incorporated in the formulation. An explicit expression is derived for the critical buckling pressure for a double-walled carbon nanotube. The influence of the small length scale on the buckling pressure is examined. It is concluded that the critical buckling pressure for a carbon nanotube could be overestimated by the classic (local) shell model due to ignoring the effect of small length scale.

Hui-Shen Shen and Chen-Li Zhang (Department of Engineering Mechanics, Shanghai Jiao Tong University, Shanghai 200030, People's Republic of China), “Nonlocal Shear Deformable Shell Model for Post-Buckling of Axially Compressed Double-Walled Carbon Nanotubes Embedded in an Elastic Matrix”, *J. Appl. Mech.*, Vol. 77, No. 4, July 2010, 041006 (12 pages), doi:10.1115/1.4000910

ABSTRACT: Buckling and post-buckling analysis is presented for axially compressed double-walled carbon nanotubes (CNTs) embedded in an elastic matrix in thermal environments. The double-walled carbon nanotube is modeled as a nonlocal shear deformable cylindrical shell, which contains small scale effects and van der Waals interaction forces. The surrounding elastic medium is modeled as a tensionless Pasternak foundation. The post-buckling analysis is based on a higher order shear deformation shell theory with the von Kármán–Donnell-type of kinematic nonlinearity. The thermal effects are also included and the material properties are assumed to be temperature-dependent and are obtained from molecular dynamics (MD) simulations. The nonlinear prebuckling deformations of the shell and the initial local point defect, which is simulated as a dimple on the tube wall, are both taken into account. A singular perturbation technique is employed to determine the post-buckling response of the tubes and an iterative scheme is developed to obtain numerical results without using any assumption on the shape of the contact region between the tube and the elastic medium. The small scale parameter e_0a is estimated by matching the buckling loads of CNTs observed from the MD simulation results with the numerical results obtained from the nonlocal shear deformable shell model. Numerical solutions are presented to show the post-buckling behavior of CNTs surrounded by an elastic medium of conventional and tensionless Pasternak foundations. The results show that buckling and post-buckling behavior of CNTs is very sensitive to the small scale parameter e_0a . The results reveal that the unilateral constraint has a significant effect on the post-buckling response of CNTs when the foundation stiffness is sufficiently large.

Hui-Shen Shen, Department of Engineering Mechanics, State Key Laboratory of Ocean Engineering, Shanghai Jiao Tong University, Shanghai, People's Republic of China. hsshshen@mail.sjtu.edu.cn, “Nonlocal shear deformable shell model for postbuckling of axially compressed microtubules embedded in an elastic medium.”, *Biomechanics and Modeling in Mechanobiology*, 2010, 9(3):345-57.

ABSTRACT: Buckling and postbuckling analysis is presented for axially compressed microtubules (MTs) embedded in an elastic matrix of cytoplasm. The microtubule is modeled as a nonlocal shear deformable cylindrical shell which contains small scale effects. The surrounding elastic medium is modeled as a Pasternak

foundation. The governing equations are based on higher order shear deformation shell theory with a von Kármán–Donnell-type of kinematic nonlinearity and include the extension-twist and flexural-twist couplings. The thermal effects are also included and the material properties are assumed to be temperature-dependent. The small scale parameter $\epsilon(0)a$ is estimated by matching the buckling load from their vibrational behavior of MTs with the numerical results obtained from the nonlocal shear deformable shell model. The numerical results show that buckling load and postbuckling behavior of MTs are very sensitive to the small scale parameter $\epsilon(0)a$. The results reveal that the MTs under axial compressive loading condition have an unstable postbuckling path, and the lateral constraint has a significant effect on the postbuckling response of a microtubule when the foundation stiffness is sufficiently large.

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“Torsional buckling and postbuckling of double-walled carbon nanotubes by nonlocal shear deformable shell model”, *Composite Structures*, Vol. 92, No. 5, April 2010, pp. 1073-1084, doi:10.1016/j.compstruct.2009.10.002

ABSTRACT: This paper presents an investigation on the buckling and postbuckling of double-walled carbon nanotubes (CNTs) subjected to torsion in thermal environments. The double-walled carbon nanotube is modeled as a nonlocal shear deformable cylindrical shell which contains small scale effects and van der Waals interaction forces. The governing equations are based on higher order shear deformation shell theory with a von Kármán–Donnell-type of kinematic nonlinearity and include the extension-twist and flexural-twist couplings. The thermal effects are also included and the material properties are assumed to be temperature-dependent and are obtained from molecular dynamics (MD) simulations. The small scale parameter $\epsilon_0 a$ is estimated by matching the buckling torque of CNTs observed from the MD simulation results with the numerical results obtained from the nonlocal shear deformable shell model. The results show that buckling torque and postbuckling behavior of CNTs are very sensitive to the small scale parameter $\epsilon_0 a$. The results reveal that the size-dependent and temperature-dependent material properties have a significant effect on the torsional buckling and postbuckling behavior of both single-walled and double-walled CNTs.

Shen, HS., Department of Engineering Mechanics, Shanghai Jiao Tong University, Shanghai 200030, People's Republic of China. hssh@mail.sjtu.edu.cn, “Buckling and postbuckling of radially loaded microtubules by nonlocal shear deformable shell model”, *J Theor Biol*, 2010 May 21; 264(2): 386-94, Epub 2010 Feb 16.

ABSTRACT: This paper presents an investigation on the buckling and postbuckling of microtubules (MTs) subjected to a uniform external radial pressure in thermal environments. The microtubule is modeled as a nonlocal shear deformable cylindrical shell which contains small scale effects. The governing equations are based on higher order shear deformation shell theory with a von Kármán–Donnell-type of kinematic nonlinearity and include the extension-twist and flexural-twist couplings. The thermal effects are also included and the material properties are assumed to be temperature-dependent. A singular perturbation technique is employed to determine the buckling pressure and postbuckling equilibrium paths. The small scale parameter $\epsilon(0)a$ is estimated by matching the buckling pressure of MTs measured from the experiments with the numerical results obtained from the nonlocal shear deformable shell model. The numerical results show that buckling pressure and postbuckling behavior of MTs are very sensitive to the small scale parameter $\epsilon(0)a$. The results reveal that the 13_3 microtubule has a stable postbuckling path, whereas the 13_2 microtubule has an unstable postbuckling behavior due to the presence of skew angles.

Chun Tang, Jeremy Feliciano, Changfeng Chen, (Department of Physics and Astronomy and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, NV 89154), “Aspect Ratio Dependant Buckling Mode Transition in Single-Walled Carbon Nanotubes under Compression”, *Bulletin of the American Physical Society*, APS March Meeting 2011, Vol. 56, No. 1, March 21–25, 2011; Dallas, Texas

ABSTRACT: We have conducted molecular dynamics simulations on compressing behaviors of single-walled carbon nanotubes (SWCNTs) with a large variety of aspect ratios. It is found that SWCNTs with large aspect ratios experience column buckling behavior at low strain levels, in contrast to commonly observed shell buckling of short SWCNTs. Further compression leads to a transition to a shell buckling mode, which is distinct from those of short SWCNTs under compression. It originates from the column buckling induced bending loadings. We extract the scaling law with respect to the aspect ratio of SWCNTs based on an analytical model of bending buckling.

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“Aspect ratio dependent buckling mode transition in single-walled carbon nanotubes under compression”, *J. Appl. Phys.*, Vol. 109, 084323 (2011); doi:10.1063/1.3569616 (5 pages)

ABSTRACT: Using molecular dynamics simulations, we study axial compressive behavior of single-walled carbon nanotubes (SWCNTs) with a wide range of aspect ratios (length to diameter ratio). It is shown that the difference in aspect ratio leads to distinct buckling modes in SWCNTs. Small-aspect-ratio SWCNTs primarily exhibit shell buckling; they switch to a column buckling mode with increasing aspect ratio. Further compression of the already column buckled large-aspect-ratio SWCNTs results in a shell buckling. This shell buckling mode is distinct from that of small-aspect-ratio SWCNTs in that it originates from the column buckling induced bending deformation. The transition strain from column buckling to shell buckling of large-aspect-ratio SWCNTs is predicted using an analytical expression. The underlying mechanism is discussed by analyzing the variation of C-C bond lengths and angles.

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“Stability analysis of carbon nanotubes using a hybrid atomistic-structural element”, *International Journal of Nanomanufacturing*, Vol. 5, Nos. 3-4, 2010, pp. 366-375, doi: 10.1504/IJNM.2010.033879

ABSTRACT: In this paper, a hybrid atomistic-structural element for studying the mechanical behaviour of carbon nanotubes is introduced. Non-linear formulation for this element is derived based on empirical inter-atomic potentials. This hybrid element is capable of taking into account the non-linear nature of inter-atomic forces as well as the non-linearity arising from large deformations. Using these capabilities, the stability analysis of carbon nanotubes under axial compressive loading is performed and the post-buckling behaviour is predicted. Also, the dependence of axial buckling force on nanotube radius is shown.

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“Nonlocal continuum theories of beams for the analysis of carbon nanotubes”, *Journal of Applied Physics*, Vol. 103, No. 2, January 2008, doi: 10.1063/1.2833431

ABSTRACT: The equations of motion of the Euler–Bernoulli and Timoshenko beam theories are reformulated using the nonlocal differential constitutive relations of Eringen [*International Journal of Engineering Science* 10, 1–16 (1972)]. The equations of motion are then used to evaluate the static bending, vibration, and buckling responses of beams with various boundary conditions. Numerical results are presented using the nonlocal theories to bring out the effect of the nonlocal behavior on deflections, buckling loads, and natural frequencies of carbon nanotubes.

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“Accurate modeling of buckling of single- and double-walled carbon nanotubes based on shell theories”, *J. Phys.: Condensed Matter* Vol. 21, No. 43, 2009, 435301, doi: 10.1088/0953-8984/21/43/435301

ABSTRACT: The accuracy of widely employed classical shell-theory-based formulae to calculate the buckling strain of single- and double-walled carbon nanotubes is assessed here. It is noted that some simplifications have been made in deriving these widely employed formulae. As a result critical buckling strains calculated from these formulae are independent of aspect ratio (length/diameter). However, molecular dynamics simulation results in the literature show an aspect ratio dependence of buckling strain. Therefore, analytical expressions are derived in this paper to calculate buckling strains of single- and double-walled carbon nanotubes based on classical shell theory without simplifications. Applicability of these expressions is further verified through molecular dynamics simulations based on the COMPASS force field. In addition, improvement in results achieved through a refinement of classical shell theory is assessed by calculating buckling strains based on first-order shell theory. Results show that simplified formulae introduce a significant error at higher aspect ratios and smaller diameters. The formulae derived here show reasonable agreement with the molecular dynamics results at all aspect ratios and diameters. First-order shell theory is found to produce a slight improvement in results for CNTs with smaller diameters and lower aspect ratios.

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“Molecular dynamics analysis on buckling of defective carbon nanotubes”, *J. Phys.: Condensed Matter*, Vol.22, 2010, 345301 doi: 10.1088/0953-8984/22/34/345301

ABSTRACT: Owing to their remarkable mechanical properties, carbon nanotubes have been employed in many diverse areas of applications. However, similar to any of the many man-made materials used today, carbon nanotubes (CNTs) are also susceptible to various kinds of defects. Understanding the effect of defects on the mechanical properties and behavior of CNTs is essential in the design of nanotube-based devices and composites. It has been found in various past studies that these defects can considerably affect the tensile strength and fracture of CNTs. Comprehensive studies on the effect of defects on the buckling and vibration of nanotubes is however lacking in the literature. In this paper, the effects of various configurations of atomic vacancy defects, on axial buckling of single-walled carbon nanotubes (SWCNTs), in different thermal environments, is investigated using molecular dynamics simulations (MDS), based on a COMPASS force field. Our findings revealed that even a single missing atom can cause a significant reduction in the critical buckling strain and load of SWCNTs. In general, increasing the number of missing atoms, asymmetry of vacancy configurations and asymmetric distribution of vacancy clusters seemed to lead to higher deterioration in

buckling properties. Further, SWCNTs with a single vacancy cluster, compared to SWCNTs with two or more vacancy clusters having the same number of missing atoms, appeared to cause higher deterioration of buckling properties. However, exceptions from the above mentioned trends could be expected due to chemical instabilities of defects. Temperature appeared to have less effect on defective CNTs compared to pristine CNTs.

Metin Aydogdu (Department of Mechanical Engineering, Trakya University, 22180 Edirne, Turkey), “A general nonlocal beam theory: Its application to nanobeam bending, buckling and vibration”, *Physica E: Low-dimensional Systems and Nanostructures*, Vol. 41, No. 9, September 2009, pp. 1651-1655, doi:10.1016/j.physe.2009.05.014

ABSTRACT: In the present study, a generalized nonlocal beam theory is proposed to study bending, buckling and free vibration of nanobeams. Nonlocal constitutive equations of Eringen are used in the formulations. After deriving governing equations, different beam theories including those of Euler–Bernoulli, Timoshenko, Reddy, Levinson and Aydogdu [*Compos. Struct.*, 89 (2009) 94] are used as a special case in the present compact formulation without repeating derivation of governing equations each time. Effect of nonlocality and length of beams are investigated in detail for each considered problem. Present solutions can be used for the static and dynamic analyses of single-walled carbon nanotubes.

S.C. Pradhan and G.K. Reddy (Department of Aerospace Engineering, Indian Institute of Technology, Kharagpur, West Bengal 721 302, India), “Buckling analysis of single walled carbon nanotube on Winkler foundation using nonlocal elasticity theory and DTM”, *Computational Materials Science*, Vol. 50, No. 3, January 2011, pp. 1052-1056, doi:10.1016/j.commatsci.2010.11.001

ABSTRACT: In the present work differential transformation method (DTM) is used to predict the buckling behaviour of single walled carbon nanotube (SWCNT) on Winkler foundation under various boundary conditions. Four different boundary conditions namely clamped–clamped, simply supported, clamped hinged and clamped free are used to study the critical buckling loads. Effects of (i) size of SWCNT (ii) nonlocal parameter and (iii) Winkler elastic modulus on nonlocal critical buckling loads are being investigated and discussed. The DTM is implemented for the nonlocal SWCNT analyses and this yields results with high degree of accuracy. Further, present method can be applied to linear and nonlinear problems.

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“Effect of strain rate on the buckling behavior of single- and double-walled carbon nanotubes”, *Carbon*, Vol.45, No. 3, March 2007, pp. 514-523, doi:10.1016/j.carbon.2006.10.020

ABSTRACT: Molecular dynamics simulations are performed on single- (SWCNTs) and double-walled carbon nanotubes (DWCNTs) to investigate the effects of strain rate on their buckling behavior. The Brenner’s second-generation reactive empirical bond order and Lennard-Jones 12-6 potentials are used to describe the short range bonding and long range van der Waals atomic (vdW) interaction within the carbon nanotubes, respectively. The sensitivity of the buckling behavior with respect to the strain rate is investigated by prescribing different axial velocities to the ends of the SWCNTs and DWCNTs in the compression simulations. In addition, the effects of vdW interaction between the walls of the DWCNTs on their buckling behavior are also examined. The simulation results show that higher strain rates lead to higher buckling loads and buckling strains for both SWCNTs and DWCNTs. A distinguishing characteristic between SWCNTs and DWCNTs is that the former experiences an abrupt drop in axial load whereas the axial load in latter decreases over a finite, albeit small,

range of strain after buckling initiates. The buckling capability of DWCNT is enhanced in the presence of vdW interaction. DWCNTs can sustain a higher strain before buckling than SWCNTs of similar diameter under otherwise identical conditions.

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“Molecular dynamics simulations on buckling of multiwalled carbon nanotubes under bending”, *J. Appl. Phys.* Vol. 100, 114327 (2006); doi:10.1063/1.2400096 (5 pages), (no doi is given)

ABSTRACT: Buckling of multiwalled carbon nanotubes (MWCNTs) subjected to bending deformation is studied using molecular dynamics simulations. We show that the initial buckling mode of a thick MWCNT is quite different from that of a thin MWCNT. Only several outer layers buckle first while the rest inner layers remain stable in a very thick MWCNT, while in a relatively thin MWCNT, all individual tubes buckle simultaneously. Such a difference in the initial buckling modes results in quite different size effects on the bending behavior of MWCNTs. In particular, the critical buckling curvature of a thick MWCNT is insensitive to the tube thickness, which is in contrast with linear elasticity. It is found also that the initial buckling wavelength is weakly dependent on the thickness of the MWCNT. We demonstrate that rippling deformation does decrease the effective modulus of a bent MWCNT, as observed in experiments. Finally, we show that the interlayer van der Waals interactions have little effect on the bending behavior of a MWCNT in the linear elastic regime.

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“The effect of intertube van der Waals interaction on the stability of pristine and functionalized carbon nanotubes under compression”, *Nanotechnology*, Vol. 21, 2010, 125704 doi: 10.1088/0957-4484/21/12/125704

ABSTRACT: This paper investigates the effect of intertube van der Waals interaction on the stability of pristine and covalently functionalized carbon nanotubes under axial compression, using molecular mechanics simulations. After regulating the number of inner layers of the armchair four-walled (5, 5)@(10, 10)@(15, 15)@(20, 20) and zigzag four-walled (6, 0)@(15, 0)@(24, 0)@(33, 0) carbon nanotubes, the critical buckling strains of the corresponding tubes are calculated. The results show that each of the three inner layers in the functionalized armchair nanotube noticeably contributes to the stability of the outermost tube, and together increase the critical strain amplitude by 155%. However, the three inner layers in the corresponding pristine nanotube, taken together, increase the critical strain of the outermost tube by only 23%. In addition, for both the pristine and functionalized zigzag nanotubes, only the (24, 0) layer, among the three inner layers, contributes to the critical strain of the corresponding outermost tube, by 11% and 29%, respectively. The underlying mechanism of the enhanced stability related to nanotube chirality and functionalization is analyzed in detail.

Xiaohu Yao and Qiang Han (Department of Engineering Mechanics, College of Traffic and Communications, South China University of Technology, Guangzhou, 510640, P.R. China), “Buckling Analysis of Multiwalled Carbon Nanotubes Under Torsional Load Coupling With Temperature Change”, *ASME J. Eng. Mater. Technol.* Vol. 128, No. 3, July 2006, pp. 419–428, doi:10.1115/1.2203102

ABSTRACT: The buckling of multiwalled carbon nanotubes under torsional load coupling with temperature

change is researched. The effects of torsional load, temperature change, surrounding elastic medium, and van der Waals forces between the inner and outer nanotubes are taken into account at the same time. Using continuum mechanics, an elastic multishell model with thermal effect is presented for buckling of a multiwalled carbon nanotube embedded in an elastic matrix under thermal environment and torsional load. Based on the model, numerical results for the general case are obtained for the thermal effect on buckling of a multiwalled carbon nanotube under torsional load. It is shown that the buckling torque of a multiwalled carbon nanotube under a certain value of temperature change is dependent on the wave number of torsional buckling modes, and a conclusion is drawn that at room or lower temperature the critical torsional load for infinitesimal buckling of a multiwalled carbon nanotube increases as the value of temperature change increases, while at temperature higher than room temperature the critical torsional load for infinitesimal buckling of a multiwalled carbon nanotube decreases as the value of temperature change increases.

Xiaohu Yao and Qiang Han (Department of Engineering Mechanics, College of Traffic and Communications, South China University of Technology, Guangzhou, 510640, PR China), "Postbuckling prediction of double-walled carbon nanotubes under axial compression", *European Journal of Mechanics - A/Solids*, Vol. 26, No. 1, January-February 2007, pp. 20-32, doi:10.1016/j.euromechsol.2006.01.008

ABSTRACT: An elastic double-shell model is presented for the buckling and postbuckling of a double-walled carbon nanotube subjected to axial compression. The analysis is based on a continuum mechanics model in which each tube of a double-walled carbon nanotube is described as an individual elastic shell and the interlayer friction is negligible between the inner and outer tubes. The governing equations are based on the Kármán–Donnell-type nonlinear differential equations. The van der Waals interaction between the inner and outer nanotubes and the nonlinear prebuckling deformations of the shell are both taken into account. A boundary layer theory of shell buckling is extended to the case of double-walled carbon nanotubes under axial compression. A singular perturbation technique is employed to determine the buckling loads and postbuckling equilibrium paths. Numerical results reveal that the single-walled carbon nanotube and the double-walled carbon nanotube both have an unstable postbuckling behavior.

H. Qian and K.Y. Xu (Shanghai Institute of Applied Mathematics and Mechanics, Department of Mechanics, Shanghai University, 99 Shangda Road, Shanghai 200444, People's Republic of China, email:

kyxu@staff.shu.edu.cn), "Curvature effects on pressure-induced buckling of empty or filled double-walled carbon nanotubes", *Acta Mechanica*, Vol. 187, Nos. 1-4, 2006, pp. 55-73, doi: 10.1007/s00707-006-0372-1

ABSTRACT: The curvature effects of interlayer van der Waals (vdW) forces on pressure-induced buckling of empty or filled double-walled carbon nanotubes (DWNTs) are studied for various radii, length-to-radius ratios, end conditions and internal-to-external pressure ratios. The analysis is based on a double-elastic shell model and assumes that the interlayer vdW pressure at a point between the inner and outer tubes depends not only on the change of the interlayer spacing, but also on the change of the curvatures of the inner and outer tubes at that point. Here the role of filling substances inside DWNTs is modeled by a uniformly distributed internal pressure. The present work aims to study the curvature effects on critical radial pressure. An explicit formula is obtained for the external buckling pressure of empty or filled DWNTs. The critical value of external pressure is estimated with various internal-to-external pressure ratios. It is shown that the curvature effects play a more significant role in buckling problems under radial pressure for small radii DWNTs than under pure axial stress. Our results show that loading transfer through vdW forces prior to buckling is important for the pressure-induced buckling of DWNTs rather than axially compressed buckling.

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kyxu@staff.shu.edu.cn), “Curvature effects on buckling of double-walled carbon nanotubes under combined axial compression and lateral pressure”, *Smart Mater. Struct.*, Vol. 16, No. 6, 2007, p. 1997
doi: 10.1088/0964-1726/16/6/002

ABSTRACT: Based on a curvature model for van der Waals (vdW) pressure between the interlayer of a double-walled carbon nanotube (DWNT), explicit expressions are derived for the critical buckling load of a DWNT which is modeled as a double-elastic shell under combined axial compression and lateral pressure. The critical load is calculated for various radii, length-to-radius ratios and load combinations. New results show that the curvature effects play a significant role in buckling problems for DWNTs of small radii. Neglecting the curvature effect usually leads to an under-estimate of the critical load for DWNTs when lateral pressure dominates. In addition, unlike Wang et al (2003b *Int. J. Solids Struct.* 40 3893) and Qian et al (2005 *Int. J. Solids Struct.* 42 5426), the buckling mode corresponding to the minimum axial buckling strain is unique, even when the lateral pressure is very small. For the DWNTs under combined axial compression and lateral pressure, the critical axial strain is reduced due to the external pressure.

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“Torsional elastic instability of double-walled carbon nanotubes”, *Carbon*, Vol. 48, No. 15, December 2010, pp.4362-4368, doi:10.1016/j.carbon.2010.07.050

ABSTRACT: In this paper, a theoretical analysis of the torsional buckling instability of double-walled carbon nanotubes (DWCNTs) and the DWCNTs embedded in an elastic medium is presented based on the continuum elastic shell model and Winkler spring model. Using the proposed theoretical approach, the influences of the aspect ratio, the buckling modes and the surrounding medium on the torsional stability are examined in detail. The simulation results show that the torsional instability of DWCNTs can occur in different buckling modes according to the aspect ratio. The van der Waals (vdW) interaction force between nanotubes reinforces the stiffness of nanoshells. Thus, the DWCNTs possess higher buckling stability than the SWCNTs without considering vdW interaction force.

Antonio Pantano, Mary C. Boyce, and David M. Parks (Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139-4307, USA), “Nonlinear Structural Mechanics Based Modeling of Carbon Nanotube Deformation”, *Phys. Rev. Lett.* Vol. 91, 145504 (2003) [4 pages],
doi: 10.1103/PhysRevLett.91.145504

ABSTRACT: A nonlinear structural mechanics based approach for modeling the structure and the deformation of single-wall and multiwall carbon nanotubes (CNTs) is presented. Individual tubes are modeled using shell finite elements, where a specific pairing of elastic properties and mechanical thickness of the tube wall is identified to enable successful modeling with shell theory. The effects of van der Waals forces are simulated with special interaction elements. This new CNT modeling approach is verified by comparison with molecular dynamics simulations and high-resolution micrographs available in the literature. The mechanics of wrinkling of multiwall CNTs are studied, demonstrating the role of the multiwalled shell structure and interwall van der Waals interactions in governing buckling and postbuckling behavior.

A. Pantano, M. C. Boyce, and D. M. Parks (Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, USA), “Mechanics of Axial Compression of Single and Multi-Wall Carbon Nanotubes”, *ASME J. Eng. Mater. Technol.*, Vol. 126, No. 3, July 2004, pp. 279 – 284,
doi:10.1115/1.1752926

ABSTRACT: A recently developed procedure for modeling the deformation of single and multi-wall carbon

nanotubes [13,14] is applied to nanotube buckling and post-buckling under axial compression. Critical features of the model, which is grounded in elastic shell theory, include identification of (a) an appropriate elastic modulus and thickness pair matching both the wall stretching and bending resistances of the single atomic layer nanotube walls, and (b) a sufficiently stiff interwall van der Waals potential to preserve interwall spacing in locally buckled MWNTs, as is experimentally observed. The first issue is illustrated by parametric buckling studies on a SWNT and comparisons to a corresponding MD simulation from the literature; results clearly indicating the inadequacy of arbitrarily assigning the shell thickness to be the equilibrium spacing of graphite planes. Details of the evolution of local buckling patterns in a nine-walled CNT are interpreted based on a complex interplay of local shell buckling and evolving interwall pressure distributions. The transition in local buckling wavelengths observed with increasing post-buckling deformation is driven by the lower energy of a longer-wavelength, multiwall deformation pattern, compared to the shorter initial wavelength set by local buckling in the outermost shell. This transition, however, is contingent on adopting a van der Waals interaction sufficiently stiff to preserve interlayer spacing in the post-buckled configuration.

N. Silvestre (Department of Civil Engineering and Architecture, IST-ICIST, Technical University of Lisbon, Av. Rovisco Pais, 1049-001 Lisbon, Portugal), “Length dependence of critical measures in single-walled carbon nanotubes”, *International Journal of Solids and Structures*, Vol. 45, Nos. 18-19, September 2008, pp. 4902-4920, doi:10.1016/j.ijsolstr.2008.04.029

ABSTRACT: This paper presents an investigation on the buckling behaviour of single-walled carbon nanotubes under various loading conditions (compression, bending and torsion) and unveils several aspects concerning the dependence of critical measures (axial strain, bending curvature and twisting angle) on the nanotube length. The buckling results are obtained by means of an atomistic-scale generalized beam theory (GBT) that incorporates local deformation of the nanotube cross-section by means of independent and orthogonal deformation modes. Moreover, some estimates are also obtained by means of non-linear shell finite element analyses using Abaqus code. After classifying the buckling modes of thin-walled tubes (global, local and distortional), the paper addresses the importance of the two-wave distortional mode (flattening or ovalization mode) in their structural behaviour. Then, the well known expression to determine the critical strain of compressed nanotubes, which is based on Donnell theory for shallow shells, is shown to be inadequate for moderately long tubes due to warping displacements appearing in the distortional buckling modes. After that, an in-depth study on the buckling behaviour of nanotubes under compression, bending and torsion is presented. The variation of the critical kinematic measures (axial strain, bending curvature and twisting angle) with the tube length is thoroughly investigated. Concerning this dependence, some uncertainties that exist in the specific literature are meticulously explained, a few useful expressions to determine critical measures of nanotubes are proposed and the results are compared with available data collected from several published works (most of them, obtained from molecular dynamics simulations).

N. Silvestre and D. Camotim (Department of Civil Engineering and Architecture, ICIST/IST, Technical University of Lisbon, Lisboa, Portugal, email: nunos@civil.ist.utl.pt), “Stability of Compressed Carbon Nanotubes Using Shell Models”, *Nanotechnology in Construction* 3, 2009, Part 3, pp. 357-363, doi: 10.1007/978-3-642-00980-8_48

ABSTRACT: This paper presents some remarks on the use of shell models to analyse the stability behaviour of single-walled NTs under compression. It is shown that there are three different categories of critical buckling modes of NTs under compression: while the axi-symmetric mode is critical for very short NTs, the flexural buckling mode is critical for long tubes. While the former exhibits cross-section contour deformation but no warping deformation, the later is characterised by the opposite situation (warping deformation but no contour deformation). Additionally, a third category exists (distortional buckling): it takes place for NTs with moderate

length, it is related to the transitional buckling behaviour between the shell (axi-symmetric mode) and the rod (flexural mode) and it is characterised by both cross-section contour deformation and warping deformation. Concerning the distortional buckling behaviour of moderately long NTs, it is also shown that the well known Donnell-type theory of shells leads to erroneous results.

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“Sanders shell model for buckling of single-walled carbon nanotubes with small aspect ratio”, *Composite Structures*, Vol. 93, No. 7, June 2011, pp. 1683-1691, doi:10.1016/j.compstruct.2011.01.004

ABSTRACT: In this paper, the buckling behaviour of single-walled carbon nanotubes (CNTs) is revisited by resorting to Donnell and Sanders shell models, which are put in parallel and shown to lead to very distinct results for CNTs with small aspect ratio (length-to-diameter). This paper demonstrates inability of the widely used Donnell shell theory while it shows the validity and accuracy of the Sanders shell theory in reproducing buckling strains and mode shapes of axially compressed CNTs with small aspect ratios. The results obtained by the later shell theory are close to molecular dynamics simulation results. The Sanders shell theory could capture correctly the length-dependent buckling strains of CNTs which the Donnell shell theory fails to achieve. In view of this study, researchers should adopt the Sanders thin shell theory from hereon instead of the Donnell theory when analyzing CNTs with small aspect ratios.

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“Prediction of buckling characteristics of carbon nanotubes”, *International Journal of Solids and Structures*, Vol. 44, No. 20, October 2007, pp. 6535-6550, doi:10.1016/j.ijsolstr.2007.02.043

ABSTRACT: In this paper, to investigate the buckling characteristics of carbon nanotubes, an equivalent beam model is first constructed. The molecular mechanics potentials in a C–C covalent bond are transformed into the form of equivalent strain energy stored in a three dimensional (3D) virtual beam element connecting two carbon atoms. Then, the equivalent stiffness parameters of the beam element can be estimated from the force field constants of the molecular mechanics theory. To evaluate the buckling loads of multi-walled carbon nanotubes, the effects of van-der Waals forces are further modeled using a newly proposed rod element. Then, the buckling characteristics of nanotubes can be easily obtained using a 3D beam and rod model of the traditional finite element method (FEM). The results of this numerical model are in good agreement with some previous results, such as those obtained from molecular dynamics computations. This method, designated as molecular structural mechanics approach, is thus proved to be an efficient means to predict the buckling characteristics of carbon nanotubes. Moreover, in the case of nanotubes with large length/diameter, the validity of Euler’s beam buckling theory and a shell model with the proper material properties defined from the results of present 3D FEM beam model is investigated to reduce the computational cost. The results of these simple theoretical models are found to agree well with the existing experimental results.

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“Computational Study of Compressive Loading of Carbon Nanotubes”, *Computational Science and Its*

Applications – ICCSA 2010, Lecture Notes in Computer Science, 2010, Volume 6017/2010, 25-43, doi: 10.1007/978-3-642-12165-4_3

ABSTRACT: A reduced-order general continuum method is used to examine the mechanical behavior of single-walled carbon nanotubes (CNTs) under compressive loading and unloading conditions. Quasi-static solutions are sought where the total energy of the system is minimized with respect to the spatial degree of freedom. We provide detailed buckled configurations for four different types of CNTs and show that, among the cases studied, the armchair CNT has the strongest resistance to the compressive loading. It is also shown that the buckled CNT will significantly lose its structural strength with the zigzag lattice structure. The unloading post-buckling of CNT demonstrates that even after the occurrence of buckling the CNT can still return to its original state making its use desirable in fields such as synthetic biomaterials, electromagnetic devices, or polymer composites.

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“Coordinated buckling of thick multi-walled carbon nanotubes under uniaxial compression”, Nano Research, Vol. 3, No. 1, 2010, pp. 32-42, doi: 10.1007/s12274-010-1005-5

ABSTRACT: Using a generalized quasi-continuum method, we characterize the post-buckling morphologies and energetics of thick multi-walled carbon nanotubes (MWCNTs) under uniaxial compression. Our simulations identify for the first time evolving post-buckling morphologies, ranging from asymmetric periodic rippling to a helical diamond pattern. We attribute the evolving morphologies to the coordinated buckling of the constituent shells. The post-buckling morphologies result in significantly reduced effective moduli that are strongly dependent on the aspect ratio. Our simulation results provide fundamental principles to guide the future design of high-performance, MWCNT-based nanodevices.

C.Q. Sun and K.X. Liu (LTCS and Department of Mechanics and Aerospace Engineering, College of Engineering, Peking University, Beijing 100871, People's Republic of China, email: kliu@pku.edu.cn), “Combined torsional buckling of multi-walled carbon nanotubes coupling with radial pressures”, J. Phys. D: Appl. Phys. Vol. 40, 2007, p. 4027, doi: 10.1088/0022-3727/40/13/018

ABSTRACT: This paper investigates the combined torsional buckling of multi-walled carbon nanotubes (MWNTs) coupling with radial pressures. The analysis is based on the continuum mechanics model, and the effect of the van der Waals interaction between adjacent tubes is taken into account. A buckling condition is derived for determining the critical shear membrane force under combined torsional buckling, which clearly indicates the role of radial pressures. The critical shear membrane force and the buckling mode are worked out for three typical MWNTs subjected to various internal pressure or external pressure. It is shown that the effect of internal pressure or external pressure on the critical shear membrane force for combined torsional buckling of MWNTs is related to the types of MWNTs. This effect is strong for thin MWNTs, moderate for thick MWNTs and small for solid MWNTs. Numerical results also indicate that the buckling mode corresponding to the critical shear membrane force of MWNTs is unique and only dependent on the structure of MWNTs. In particular, for combined torsional buckling of MWNTs with very small internal pressure or external pressure, the buckling mode is just that for the corresponding pure torsional buckling.

C.Q. Sun and K.X. Liu (LTCS and Department of Mechanics and Aerospace Engineering, College of Engineering, Peking University, Beijing 100871, People's Republic of China, email: kliu@pku.edu.cn), “Combined torsional buckling of multi-walled carbon nanotubes coupling with radial pressures”, International

Journal of Solids and Structures, Vol. 45, Nos. 7-8, April 2008, pp. 2128-2139
doi:10.1016/j.jsoistr.2007.11.00

ABSTRACT: This paper reports the results of an investigation on combined torsional buckling of multi-walled carbon nanotubes (MWNTs) under combined torque, axial loading and radial pressures based on the continuum mechanics model, which takes into account the effect of the van der Waals interaction between adjacent tubes. A buckling condition is derived for determining the critical buckling torque and associated buckling mode. In particular, for combined torsional buckling of double-walled carbon nanotubes, an explicit expression is obtained and some detailed results are demonstrated. According to the innermost radius-to-thickness ratio, MWNTs are classified into three types: thin, thick, and (almost) solid. Numerical results are worked out for the critical buckling torque and associated buckling mode for all the three types of MWNTs subjected to various axial stresses (axial tensile stresses or axial compressive stresses), internal pressures, and external pressures. It is shown that, the axial tensile stress or the internal pressure will make the MWNTs resist higher critical buckling torque, while the axial compressive stress or external pressure will lead to a lower critical buckling torque. The effect of axial stress (axial tensile stress or axial compressive stress) on the critical buckling torque of MWNTs is very small for all the three types of MWNTs, while the effect of the internal pressure or external pressure is related to the types of MWNTs, which is strong for the thin MWNTs, moderate for the thick MWNTs, and small for the solid MWNTs. Numerical results also indicate that, the associated buckling mode is unique and dependent on the structure of MWNTs. Especially, for combined torsional buckling of MWNTs with very small axial stress and radial pressures, the buckling mode is just the one for the corresponding pure torsional buckling.

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“Torsional buckling of multi-walled carbon nanotubes under combined axial and radial loadings”, J. Phys. D: Appl. Phys. Vol. 41, 2008, p. 205404, doi: 10.1088/0022-3727/41/20/205404

ABSTRACT: This paper investigates the torsional buckling of multi-walled carbon nanotubes under combined axial and radial loadings based on the continuum mechanics model. In particular, an explicit expression is obtained for the torsional buckling of double-walled carbon nanotubes (DWNTs) under combined loadings. Numerical results show that axial tensile stress or internal pressure will make DWNTs resist higher critical shear membrane force, while axial compressive stress or external pressure will lead to a lower critical shear membrane force. Further, for torsional buckling of DWNTs coupling with small axial stress and internal pressure or external pressure, the effect of the axial stress, internal pressure or external pressure on the critical shear membrane force is linear, and the associated buckling wave numbers are unique and the same as that under corresponding pure torque.

Tianshong Chang (Shanghai Institute of Applied Mathematics and Mechanics, Shanghai University, Shanghai 200072, People's Republic of China), “Torsional behavior of chiral single-walled carbon nanotubes is loading direction dependent”, Appl. Phys. Lett. Vol. 90, p. 201910 (2007); doi:10.1063/1.2739325 (3 pages)

ABSTRACT: The torsion of carbon nanotubes is studied by molecular dynamics simulations. The torsional behavior of a chiral single-walled carbon nanotube (SWCNT) is dependent on the loading directions due to its structural asymmetry. The critical buckling shear strain of a SWCNT in one direction may be 1.8 times higher than that in the opposite direction. This means that one can choose the most appropriate SWCNT for his special purpose in designing a torsional component (e.g., oscillators and springs) of nanomechanical devices using carbon nanotubes. Meanwhile, the finding indicates that a simple thin shell model is not suitable for predicting torsional behavior of small SWCNTs at large strains.

Riaz, M., Fulati, A., Amin, G., Alvi, N. H., Nur, O., Willander, M. (Department of Science and Technology, Campus Norrköping, Linköping University, SE-601 74 Norrköping, Sweden), “Buckling and elastic stability of vertical ZnO nanotubes and nanorods”, *Journal of Applied Physics*, Vol. 106, No. 3, August 2009, pp. 034309-034309-6, doi: 10.1063/1.3190481

ABSTRACT: Buckling and elastic stability study of vertical well aligned ZnO nanorods grown on Si substrate and ZnO nanotubes etched from the same nanorods was done quantitatively by nanoindentation technique. The critical load, modulus of elasticity, and flexibility of the ZnO nanorods and nanotubes were observed and we compared these properties for the two nanostructures. It was observed that critical load of nanorods (2890 microN) was approximately five times larger than the critical load of the nanotubes (687 microN). It was also observed that ZnO nanotubes were approximately five times more flexible (0.32 nm/microN) than the nanorods (0.064 nm/microN). We also calculated the buckling energies of the ZnO nanotubes and nanorods from the force displacement curves. The ratio of the buckling energies was also close to unity due to the increase/decrease of five times for one parameter (critical load) and increase/decrease of five times for the other parameter (displacement) of the two samples. We calculated critical load, critical stress, strain, and Young modulus of elasticity of single ZnO nanorod and nanotube. The high flexibility of the nanotubes and high elasticity of the ZnO nanorods can be used to enhance the efficiency of piezoelectric nanodevices. We used the Euler buckling model and shell cylindrical model for the analysis of the mechanical properties of ZnO nanotubes and nanorods.

Tong, F. M., Wang, C. Y. and Adhikari, S. (School of Engineering, Swansea University, Singleton Park, Swansea, Wales SA2 8PP, United Kingdom), “Axial buckling of multiwall carbon nanotubes with heterogeneous boundaries”, *Journal of Applied Physics*, Vol. 105, No. 9, June 2009, pp. 094325-094325-7, doi: 10.1063/1.3125312

ABSTRACT: The finite element method has been employed to study the effects of different boundary conditions on the axial buckling of multiwall carbon nanotubes (MWCNTs). Unlike previous works, both homogeneous and heterogeneous end constraints are considered for the constituent tubes of various MWCNTs comprising shell-type (i.e., the length-to-diameter ratio $L/D \geq 10$), beam-type (i.e., $L/D < 10$), and the two different types of constituent tubes. The results show that clamping the individual tubes of simply supported or free MWCNTs exerts a variety of influences on their buckling behaviors depending on the type of the MWCNTs, the position, and the number of the clamped tubes. Clamping the outermost tube can enhance the critical buckling strain up to four times of its original value and can shift the buckling modes of those MWCNTs consisting both shell- and beam-type tubes. In contrast, little difference can be observed when simply supported ends of MWCNTs are replaced by free ends or vice versa. Explicit buckling mode shapes obtained using the finite element method for various physically realistic cases have been shown in the paper.

M. Arroyo and T. Belytschko (Department of Mechanical Engineering, Northwestern University, Evanston, Illinois 60208, USA, email: tedbelytschko@northwestern.edu), “Finite element methods for the non-linear mechanics of crystalline sheets and nanotubes”, *International Journal for Numerical Methods in Engineering*, Vol. 59, No. 3, January 2004, pp. 419–456, doi: 10.1002/nme.944

ABSTRACT: The formulation and finite element implementation of a finite deformation continuum theory for the mechanics of crystalline sheets is described. This theory generalizes standard crystal elasticity to curved monolayer lattices by means of the exponential Cauchy–Born rule. The constitutive model for a two-dimensional continuum deforming in three dimensions (a surface) is written explicitly in terms of the underlying atomistic model. The resulting hyper-elastic potential depends on the stretch and the curvature of the surface, as well as on internal elastic variables describing the rearrangements of the crystal within the unit cell. Coarse grained calculations of carbon nanotubes (CNTs) are performed by discretizing this continuum

mechanics theory by finite elements. A smooth discrete representation of the surface is required, and subdivision finite elements, proposed for thin-shell analysis, are used. A detailed set of numerical experiments, in which the continuum/finite element solutions are compared to the corresponding full atomistic calculations of CNTs, involving very large deformations and geometric instabilities, demonstrates the accuracy of the proposed approach. Simulations for large multi-million systems illustrate the computational savings which can be achieved.

M. Arroyo and T. Belytschko (Department of Mechanical Engineering, Northwestern University, Evanston, Illinois 60208, USA), “Finite crystal elasticity of carbon nanotubes based on the exponential Cauchy-Born rule”, *Phys. Rev. B*, Vol. 69, 115415 (2004) [11 pages], doi: 10.1103/PhysRevB.69.115415

ABSTRACT: A finite deformation continuum theory is derived from interatomic potentials for the analysis of the mechanics of carbon nanotubes. This nonlinear elastic theory is based on an extension of the Cauchy-Born rule called the exponential Cauchy-Born rule. The continuum object replacing the graphene sheet is a surface without thickness. The method systematically addresses both the characterization of the small strain elasticity of nanotubes and the simulation at large strains. Elastic moduli are explicitly expressed in terms of the functional form of the interatomic potential. The expression for the flexural stiffness of graphene sheets, which cannot be obtained from standard crystal elasticity, is derived. We also show that simulations with the continuum model combined with the finite element method agree very well with zero temperature atomistic calculations involving severe deformations.

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“Continuum Mechanics Modeling and Simulation of Carbon Nanotubes”, *Meccanica*, Vol. 40, Nos. 4-6, 2005. pp. 455-469, doi: 10.1007/s11012-005-2133-y

ABSTRACT: The understanding of the mechanics of atomistic systems greatly benefits from continuum mechanics. One appealing approach aims at deductively constructing continuum theories starting from models of the interatomic interactions. This viewpoint has become extremely popular with the quasicontinuum method. The application of these ideas to carbon nanotubes presents a peculiarity with respect to usual crystalline materials: their structure relies on a two-dimensional curved lattice. This renders the cornerstone of crystal elasticity, the Cauchy-Born rule, insufficient to describe the effect of curvature. We discuss the application of a theory which corrects this deficiency to the mechanics of carbon nanotubes (CNTs). We review recent developments of this theory, which include the study of the convergence characteristics of the proposed continuum models to the parent atomistic models, as well as large scale simulations based on this theory. The latter have unveiled the complex nonlinear elastic response of thick multiwalled carbon nanotubes (MWCNTs), with an anomalous elastic regime following an almost absent harmonic range.

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“Transition states and minimum energy pathways for the collapse of carbon nanotubes”, *Phys. Rev. B* 73, 075423 (2006) [7 pages], doi: 10.1103/PhysRevB.73.075423

ABSTRACT: Carbon nanotubes (CNTs) can undergo collapse from their customary cylindrical configurations to ribbons. The energy minima corresponding to these two states are identified using either atomistic molecular mechanics or the theory of finite crystal elasticity with reduced dimensionality. The minimum energy path between these two minima is found using the nudged elastic band reaction-pathway sampling scheme. The energetics of CNT collapse is explored for both single- and multi-walled CNTs as well as small bundles. The process has a strong diameter dependence, with collapse being more favorable for the larger diameter tubes, but is nearly independent of chirality. The saddle point always lies close to the collapsed state, and the absolute barrier energies—even for fairly short tube lengths—are sufficiently high, even when the reaction is highly exothermic, that thermal activation cannot initiate collapse via this pathway. The hydrostatic pressure required to buckle and collapse CNTs of various diameters is discussed.

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“Size Dependence of the Thin-Shell Model for Carbon Nanotubes”, *Phys. Rev. Lett.* 95, 105501 (2005) [4 pages], doi: 10.1103/PhysRevLett.95.105501

ABSTRACT: There has been much debate on the choice for the representative wall thickness for the thin-shell model, although this model has demonstrated remarkable success in capturing many types of behavior of single-walled carbon nanotubes (SWNTs), in determining the buckling strains under compression, torsion, and bending, in particular. This analysis, using the Tersoff-Brenner potential and ab initio calculations, shows that the elasticity of the model thin shell evolves from isotropic to square symmetric with the decreasing tube diameter, leading to significant diameter dependence for all the elastic moduli and the representative wall thickness. Furthermore, the elastic moduli of multiwalled carbon nanotubes of diameters up to 10 nm are also size dependent.

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“Can a single-wall carbon nanotube be modeled as a thin shell?”, *Journal of the Mechanics and Physics of Solids*, Vol. 56, No. 6, June 2008, pp. 2213-2224, doi:10.1016/j.jmps.2008.01.004

ABSTRACT: Single-wall carbon nanotubes (SWCNT) have been frequently modeled as thin shells, but the shell thickness and Young's modulus reported in literatures display large scattering. The order of error to approximate SWCNTs as thin shells is studied in this paper via an atomistic-based finite-deformation shell theory, which avoids the shell thickness and Young's modulus, but links the tension and bending rigidities directly to the interatomic potential. The ratio of atomic spacing (Δ approximately equal to 0.14 nm) to the radius of SWCNT, Δ/R , which ranges from zero (for graphene) to 40% [for a small (5,5) armchair SWCNT ($R=0.35$ nm)], is used to estimate the order of error. For the order of error $O[(\Delta/R)^3]$, SWCNTs cannot be represented by a conventional thin shell because their constitutive relation involves the coupling between tension and curvature and between bending and strain. For the order of error $O[(\Delta/R)^2]$, the tension and bending (shear and torsion) rigidities of SWCNTs can be represented by an elastic orthotropic thin shell, but the thickness and elastic modulus cannot. Only for the order of error $O(\Delta/R)$, a universal constant shell thickness can be defined and SWCNTs can be modeled as an elastic isotropic thin shell.

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“TEM observations of buckling and fracture modes for compressed thick multiwall carbon nanotubes”, Carbon, Vol. 49, No. 1, January 2011, pp. 206-213, doi:10.1016/j.carbon.2010.09.005

ABSTRACT: The buckling and fracture modes of thick (diameter >20 nm) multiwall carbon nanotubes (MWCNTs) under compressive stress were examined using in situ transmission electron microscopy. The overall dynamic deformation processes of the MWCNTs as well as the force/distance curves can be obtained. The buckling behavior of MWCNTs under compression falls into two categories, the first is non-axial buckling and subsequently complex Yoshimura patterns can be induced on the compressive side of the MWCNTs. The second is axial buckling followed by catastrophic failure. We find the buckling mode of thick MWCNTs is highly dependent on the diameter and length of the MWCNTs. A continuum mechanics model is employed to determine the buckling mode criterion for the MWCNTs. Moreover, the shell by shell fracture mode and planar fracture mode of MWCNTs are directly observed in our experiments.