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Prediction of the critical buckling load of multi-walled carbon nanotubes under axial compression

Prédiction de la charge critique de flambage des nanotubes de carbone multi-parois sous compression axiale

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ABSTRACT

In this paper, we propose a new explicit analytical formula of the critical buckling load of double-walled carbon nanotubes (DWCNT) under axial compression. This formula takes into account van der Waals interactions between adjacent tubes and the effect of terms involving tube radii differences generally neglected in the derived expressions of the critical buckling load published in the literature. The elastic multiple Donnell shells continuum approach is employed for modelling the multi-walled carbon nanotubes. The validation of the proposed formula is made by comparison with a numerical solution. The influence of the neglected terms is also studied.

RÉSUMÉ

Cet article a pour objectif la proposition d'une formule analytique explicite de la charge critique de flambage des nantubes de carbone à double parois (DWCNT) soumis à une compression axiale. Cette formule prend en compte les interactions de van der Waals entre les tubes adjacents et l'influence des rayons, généralement negligée dans les formules donnant la charge critique de flambage publiées dans la littérature. L'approche continue des coques multiples de Donnell est utilisée pour la modélisation des nanotubes de carbone multi-parois. La validation de la formule proposée est faite par une comparaison avec une solution numérique. L'effet des termes négligés a aussi été étudié.

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1. Introduction

Carbon nanotubes are tubular carbon molecules of diameters of a few tens of nanometers and of a length of several microns. These ultra-fine tubular carbon structures exhibit superior mechanical, electronic and thermal properties and have potential applications in nano-technology and nano-electronics. Since their discovery by Iijima in 1991 [1], carbon nanotubes have led to several innovations in nano-technology and caused profound impacts on almost all existing industries ranging from medicine, agriculture, environment and biotechnology to information technology, aeronautics, and energy. The performance of the new materials based on carbon nanotubes depends essentially on their outstanding mechanical properties.

Several research studies have been conducted to determine these properties in order to better understand their various static and dynamic behaviors such as rupture, vibration, wave propagation, and in particular their buckling behavior.

In view of their high aspect ratio and their very thin hollow cylindrical geometry, buckling of carbon nanotubes has become a very important attractive topic of research in the community of scientists who are interested in studying the instability phenomena of carbon nanotubes.

Buckling analysis of carbon nanotubes, observed in recent works, is performed using two methods: molecular dynamics simulations (classical molecular dynamics tight molecular dynamics and ab initio) and methods based on continuous models of beams, shells and truss of the continuum media mechanics. The applicability of continuum mechanics for analyzing the mechanical behavior of carbon nanotubes (CNTs) has been suggested in 1996 by Yakobson et al. [2]. Since this date, great efforts have been devoted, using the continuum mechanics approaches [3–6], to explore and simulate the buckling instability of single and multi-walled carbon nanotubes. The buckling of carbon nanotubes with single or multi walls axially compressed has been the subject of many works [7–13] based on mono- or multi-Euler–Bernoulli or Timoshenko beams [14] and Donnell or Sanders cylindrical circular-shell elastic continuum models [15–17].

The beam continuum model is valid for slender long CNTs. The buckling in this case is global. However, when the CNTs are short and have large diameters, their buckling is local and their modelling is better using shell continuum approaches. During the last recent years, buckling of double-walled carbon nanotubes (DWCNTs) under axial compression with simply supported ends is intensively studied using Donnell's cylindrical continuum shell model, taking into account van der Walls forces between the layers [7,11,12,18–20].

Analytical formulae for the buckling load of DWCNTs have been derived in the literature. These proposed formulae are based on approximations consisting in neglecting the terms involving the difference between the radii of the inner and outer tubes. Furthermore, the critical buckling load is always obtained numerically [7,11,12,18].

The aim of this paper is to propose a new explicit analytical formula for the critical buckling load of DWCNTs under axial compression for fixed aspect ratios without any assumption on radii tubes. This expression is obtained using Donnell's cylindrical continuum model taking into account the van der Waals interaction. The critical buckling load is derived by an analytical minimization procedure. A comparison with numerical result is performed to validate the proposed formula. The effect of omitting terms on the critical buckling load is also investigated.

2. Basic equations

Thin-shell theories based on continuum mechanics have been successfully applied to predict several mechanical properties of single and multi-walled carbon nanotubes (SWCNTs, DWCNTs). The Donnell elastic shell models have been applied to single-walled and multi-walled carbon nanotubes [7,8,18,19,21–25].

2.1. Donnell's cylindrical elastic shell continuum model

Consider an axially compressed buckling of a single circular cylindrical elastic shell of radius R, thickness h, Young's modulus E and Poisson's ratio ν. The equilibrium equation of the shell is given by [3,4,26–28]:

$$k^2\Delta^2 w-\rho\frac{N_y}{Eh}-\frac{1}{Eh}\left(N_x\frac{\partial^2 w}{\partial x^2}+2N_{xy}\frac{\partial^2 w}{\partial x\partial y}+N_y\frac{\partial^2 w}{\partial y^2}\right)-\frac{p}{Eh}=0 \qquad (1)$$

where $k^2=D/Eh$; with $D=Eh^3/12(1-\nu^2)$ is the bending stiffness of the shell, $\rho=1/R$ is the curvature, w is the radial displacement of the middle area, $N_x=K(\epsilon_{xx}+\nu\epsilon_{yy})$ is the axial membrane force, $N_y=K(\epsilon_{yy}+\nu\epsilon_{xx})$ is the circumferential membrane force, $N_{xy}=K(1-\nu)\epsilon_{xy}$ is the shear membrane force, p is the total radial pressure, ϵ_{xx}, ϵ_{yy} and ϵ_{xy} are the strains, x and y denote the axial and circumferential coordinates of the shell respectively, $w(x,y)$ is the radial displacement of the middle surface of the shell along the normal direction, $\Delta^2(.)=\left(\frac{\partial^2(.)}{\partial x^2}+\frac{\partial^2(.)}{\partial y^2}\right)^2$ is the bi-Laplacian operator and $K=Eh/(1-\nu^2)$.

To investigate the possible existence of adjacent equilibrium configurations, we use the adjacent equilibrium criterion [3,29]. We examine the two adjacent configurations represented by the displacements before and after increments, as follows:

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