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A continuum elastic three-dimensional model for natural frequencies of single-walled carbon nanotubes

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ABSTRACT

The free vibration analysis of Single-Walled Carbon NanoTubes (SWCNTs) is proposed in the present paper. A continuum approach (based on an exact elastic three-dimensional shell model) is used for natural frequency investigation of simply supported SWCNTs. In order to apply this continuum model, carbon nanotubes are defined as isotropic cylinders with an equivalent thickness and Young modulus. Preliminary remarks are proposed concerning the possible use of a continuum approach and the most convenient definitions of the equivalent thickness and Young modulus. Subsequently, the 3D shell method is compared with different beam analyses to show the limitations of 1D beam models. Finally, zigzag, armchair and general chirality SWCNTs (with various lengths and geometries) are analyzed via the 3D shell model to calculate their vibration modes.

1. Introduction

Carbon NanoTubes (CNTs) were discovered in Japan by Iijma [1] in 1991. CNTs are closed graphene sheets with a cylindrical shape. Research has shown that carbon nanotubes exhibit exceptional mechanical properties [2]. The elastic modulus has been shown to be greater than 1 TPa and the tensile strength exceeds that of steel by over one order of magnitude. In view of their exceptional mechanical properties, CNTs are considered to be ideal reinforcements in composite structures [3]. Most CNT applications depend on their exceptional elastic properties. Therefore, it is of central importance to accurately quantify the elastic properties of Single-Walled CNTs (SWCNTs) [4] when a continuum elastic model is applied for their analysis.

Three basic methods are used to simulate the behavior of CNTs [5]: Molecular Dynamics (MD) simulations, atomistic-based modeling approaches and continuum approaches. In the former, the simulations are based on the definition of a potential energy function (e.g., Tersoff–Brenner or Lennard–Jones functions) [6–11]. In the second approach, CNTs are investigated using an atomistic finite element model with beam elements and concentrated masses. The beams simulate the interatomic covalent forces and the masses are located at the ends of the beams and represent the carbon positions [12–17]. The third approach considers carbon nanotubes (which have a discrete molecular structure) as continuum isotropic elastic cylinders which can be analyzed via beam or shell models. The computational effort necessary for the MD approach does not allow fast simulations of complex CNT networks. Simulations of a real size multi-walled CNT by means of an atomistic-based modeling approach are also expensive. Consequently, continuum approaches are preferred to MD and atomistic-based models in the described simulations because the computational cost is better. A carbon nanotube has a discrete molecular structure. Therefore, in order to apply a continuum model, it is necessary to correctly suppose its effective wall thickness, Young modulus and Poisson ratio. Extensive studies [18–21] have been conducted to analyze this feature, but a final conclusion has not yet been reached. In fact, the thickness and Young modulus values shown in the papers analyzed below are very different for the same elastic stiffness considered.

Many researchers have used beam models for continuum approaches to analyze free vibrations of single-walled carbon nanotubes. Among these, Araújo dos Santos [22] used finite elements based on the Euler–Bernoulli and Timoshenko beam theories. Azrar et al. [23] proposed the Timoshenko beam model with generalized boundary conditions in order to take into account a more realistic and wider range of boundary conditions. Unlike the Euler–Bernoulli beam model, the Timoshenko beam model allows for the effects of transverse shear deformation and rotary inertia [24]. The discrete singular convolution (DSC) method based on the Timoshenko beam theory was used in [25] for free vibration problems of carbon nanotubes. Foda [26] proposed a direct analytical approach to suppress the steady state vibrations of a nanotube

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resting on a Winkler foundation. The natural frequencies and transversal responses of simply supported single-walled carbon nanotubes were analyzed in [27] by means of the Timoshenko beam theory and the Bernoulli–Fourier method. Ming and Huiming [28] developed a single beam model to analyze the thermal vibration of SWCNTs. In this work nonlocal elasticity incorporated the effects of small size into the formulation. The flexural vibration of single-walled carbon nanotubes was analyzed in [29] by the finite element method. The Timoshenko beam element formulation was used for this purpose. Based on the nonlocal continuum theory, the nonlinear vibration of a SWCNT (considered as a curved beam subjected to a harmonic load) was investigated in [30]. Vibrations of nanotubes embedded in an elastic matrix were investigated in [31] by using the nonlocal Timoshenko beam model. Both a stress gradient and a strain gradient approach were considered. The transverse vibration of a single-walled carbon nanotube with light waviness along its axis was modeled in [32] by the nonlocal Euler–Bernoulli and Timoshenko beam theories. The comparison between the two models shows that the effects of transverse shear deformation and rotary inertia are considered only in the Timoshenko beam model. The nonlocal Euler–Bernoulli beam theory was used in [33] for forced vibrations of a simply supported single-walled carbon nanotube subjected to a moving harmonic load. Murmu and Pradhan [34] developed a nonlocal elasticity and through the Timoshenko beam theory investigated the stability response of a SWCNT embedded in an elastic medium. For the first time, both Winkler-type and Pasternak-type foundation models were employed to simulate the interaction of the SWCNT with the surrounding elastic medium. Non-local constitutive equations of Eringen were used in [35], different beam theories including those of Euler–Bernoulli, Timoshenko, Reddy, Levinson and Aydogdu were compared.

The papers concerning the use of shell models for the vibration analysis of SWCNTs are less numerous than those concerning the beam models. Shell models are usually more complicated than beam models but they allow the analysis of CNTs with low length/diameter ratios. For these structures the use of 1D beam models gives significant errors because short CNTs are not one-dimensional structures. 2D or 3D shell models are suitable for the analysis of short CNTs. When the radius/thickness ratio is small, the use of refined 2D or 3D shell models are necessary for a correct vibration analysis as demonstrated in Cinefra et al. [36]. Wang and Zhang [37] proposed a two-dimensional elastic shell model to characterize the deformation of single-walled carbon nanotubes using the in-plane rigidity, Poisson ratio, bending rigidity and off-plane torsion rigidity as independent elastic constants. An elastic shell model of single-walled carbon nanotubes can be established only with a well-defined effective thickness. Vibrations of single-walled carbon nanotubes based on a three-dimensional theory of elasticity were analyzed in [38]. The Flügge type shell equations (including the initial membrane hoop and axial stresses) were used in [39] as governing equations for free axisymmetric vibrations of a single-walled carbon nanotube. Dong et al. [40] presented an analytical laminated cylindrical shell method to investigate wave propagation in individual multiwall carbon nanotubes (MWNTs) or MWNTs embedded in an elastic matrix. Further shell models for Double-Walled Carbon NanoTubes (DWCNTs) were proposed in [41] and in [42] for free vibration and buckling analysis, respectively.

An exact three-dimensional elastic shell model is proposed in the present paper for free vibration analysis of simply supported SWCNTs. The equilibrium equations in general orthogonal curvilinear coordinates (see [43,44]) are developed for the case of a cylinder by giving an infinite value for one of the two radii of curvature. These equations are exactly solved by imposing harmonic forms for displacement components. The present model is validated by means of a comparison with the beam models given in [33,35]. Different length/diameter ratios are analyzed to understand the limitations of 1D beam models. Afterwards, the 3D shell model is used for the analysis of vibration modes of different zigzag, armchair and general chirality SWCNTs. Particular attention is given to the definition of the equivalent elastic properties of CNTs which actually are discrete molecular structures.

2. 3D shell model

The three differential equations of equilibrium written for the case of free vibration analysis of multilayered spherical shells with constant radii of curvature R_α and R_β have been proposed in [43,44] where they have been solved in exact form in analogy with the method proposed in [45,46]. In this paper, the equations are simplified for the cylindrical case by imposing an infinite value for the radius of curvature R_β (see Fig. 1). The general form proposed in [43,44] remains valid for both plate and constant radius shell geometries.

2.1. Constitutive and geometrical relations

Three-dimensional linear elastic constitutive equations in orthogonal curvilinear coordinates (α, β, z) (see Fig. 1) are here given for a generic k isotropic layer. The stress components $(\sigma_{\alpha\alpha}, \sigma_{\beta\beta}, \sigma_{zz}, \sigma_{\beta z}, \sigma_{\alpha z}, \sigma_{\alpha\beta})$ are linked with the strain components $(\epsilon_{\alpha\alpha}, \epsilon_{\beta\beta}, \epsilon_{zz}, \gamma_{\beta z}, \gamma_{\alpha z}, \gamma_{\alpha\beta})$ for each k isotropic layer as:

$$\sigma_{\alpha\alpha k} = C_{11k}\epsilon_{\alpha\alpha k} + C_{12k}\epsilon_{\beta\beta k} + C_{13k}\epsilon_{zzk}, \tag{1}$$

$$\sigma_{\beta\beta k} = C_{12k}\epsilon_{\alpha\alpha k} + C_{22k}\epsilon_{\beta\beta k} + C_{23k}\epsilon_{zzk}, \tag{2}$$

$$\sigma_{zzk} = C_{13k}\epsilon_{\alpha\alpha k} + C_{23k}\epsilon_{\beta\beta k} + C_{33k}\epsilon_{zzk}, \tag{3}$$

$$\sigma_{\beta zk} = C_{44k}\gamma_{\beta zk}, \tag{4}$$

$$\sigma_{\alpha zk} = C_{55k}\gamma_{\alpha zk}, \tag{5}$$

$$\sigma_{\alpha\beta k} = C_{66k}\gamma_{\alpha\beta k}. \tag{6}$$

The strain–displacement relations of three-dimensional theory of elasticity in orthogonal curvilinear coordinates are written for the generic k layer of the multilayered cylindrical shell of Fig. 1 (the general form for spherical shells with constant radii of curvature R_α and R_β has been given in [43,44]):

$$\epsilon_{\alpha\alpha k} = \frac{1}{H_\alpha}u_{k,\alpha} + \frac{w_k}{H_\alpha R_\alpha}, \tag{7}$$

$$\epsilon_{\beta\beta k} = v_{k,\beta}, \tag{8}$$

$$\epsilon_{zzk} = w_{k,z}, \tag{9}$$

$$\gamma_{\beta zk} = w_{k,\beta} + v_{k,z}, \tag{10}$$

$$\gamma_{\alpha zk} = \frac{1}{H_\alpha}w_{k,\alpha} + u_{k,z} - \frac{u_k}{H_\alpha R_\alpha}, \tag{11}$$

$$\gamma_{\alpha\beta k} = \frac{1}{H_\alpha}v_{k,\alpha} + u_{k,\beta}. \tag{12}$$

The parametric coefficients for cylindrical shells are:

$$H_\alpha = \left(1 + \frac{z}{R_\alpha}\right), \quad H_\beta = 1, \quad H_z = 1, \tag{13}$$

H_α depends on the z coordinate. $H_\beta = 1$ and $H_z = 1$ because β and z are rectilinear coordinates. R_α is the principal radius of curvature along the α coordinate. R_β is infinite for a cylinder (see Fig. 1). Partial derivatives $\frac{\partial}{\partial\alpha}$, $\frac{\partial}{\partial\beta}$ and $\frac{\partial}{\partial z}$ are indicated with subscripts $(,\alpha)$, $(,\beta)$ and $(,z)$.

2.2. Equilibrium equations

The three differential equations of equilibrium written for the case of free vibration analysis of cylindrical shells are given (the