Mechanics of Advanced Materials and Structures
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/umcm20

Refined Shell Models for the Vibration Analysis of Multiwalled Carbon Nanotubes

M. Cinefra [a b c], E. Carrera [a] & S. Brischetto [a]

[a] Department of Aeronautics and Space Engineering, Politecnico di Torino, Torino, Italy

[b] CRP H. Tudor, Esch-sur-Alzette, Luxembourg

[c] Department LMpX, Universitéé Paris X, France

Available online: 27 Sep 2011

To cite this article: M. Cinefra, E. Carrera & S. Brischetto (2011): Refined Shell Models for the Vibration Analysis of Multiwalled Carbon Nanotubes, Mechanics of Advanced Materials and Structures, 18:7, 476-483

To link to this article: http://dx.doi.org/10.1080/15376494.2011.604601

Mechanics of Advanced Materials and Structures, 18:476–483, 2011

ISSN: 1537-6494 print / 1537-6532 online
DOI: 10.1080/15376494.2011.604601

Taylor & Francis
Taylor & Francis Group

Refined Shell Models for the Vibration Analysis of Multiwalled Carbon Nanotubes

M. Cinefra,[1,2,3] E. Carrera,[1] and S. Brischetto[1]

[1]*Department of Aeronautics and Space Engineering, Politecnico di Torino, Torino, Italy*
[2]*CRP H. Tudor, Esch-sur-Alzette, Luxembourg*
[3]*Department LMpX, Université Paris X, France*

The free vibration response of double-walled carbon nanotubes is studied in this article. A continuum approach is used and refined shell models are obtained through the application of Carrera's Unified Formulation (CUF). In order to apply the continuum models, the multi-walled carbon nanotube is assumed to be a multilayer cylindrical shell with an equivalent thickness and Young's modulus. Equivalent single-layer and layer-wise approaches in CUF are modified to consider the nested tubes of a multi-walled carbon nanotube as independent and separately vibrating. The van der Waals interaction between two adjacent tubes is estimated by using the Lennard-Jones model. The proposed results emphasize the differences that exist among available continuum models and present shell approaches. In particular, the attention is devoted to van der Waals interaction and a comparison has been made between models that take into account the van der Waals forces and models that neglect them.

Keywords Uniformed Formulation, continuum shell models, vibration analysis, double-walled carbon nanotubes, van der Waals forces

1. INTRODUCTION

Much research has been carried out on carbon nanotubes (CNTs) since their discovery in Japan by Iijima [1] in 1991. Carbon nanotubes exhibit superior mechanical properties and are extremely promising due to their strong, light, and high toughness characteristics.

Two basic methods are used to simulate the mechanical behavior of nanostructures: atomistic-based modelling approaches and continuum approaches. In the former, the vibrational behavior of CNTs is investigated using an atomistic finite element model with beam elements and concentrated masses [2, 3]. The beams simulate the interatomic covalent forces and the masses are located at the ends of the beams and represent the carbon position: the computational effort necessary for these methods does not permit simulations of real size multi-walled CNTs. For these reasons, continuum approaches are preferred to atomistic-based ones.

A carbon nanotube has a discrete molecular structure, therefore, it is necessary to know its effective wall thickness and calculate its effective Young's modulus in order to apply a continuum model. Inspired by these motivations, extensive studies [4–9] have been conducted over the past ten years to examine the above-mentioned issues. Unfortunately, considerable inconsistence has been found in the literature, where the values obtained for the same elastic stiffness and the effective wall thickness are very different. Since the aim of the present article is to demonstrate the efficiency of the shell models contained in the CUF for the analysis of carbon nanotubes, the single-walled carbon nanotube (SWCNT) is considered as an isotropic elastic thin shell with wall thickness h equal to the interplanar spacing of graphite layers, according to the most common assumption in the literature.

In the literature, many researchers have used beam models to analyze the mechanical behavior of carbon nanotubes. Among these, Wang et al. [10] and Aydogdu [11, 12] have studied the vibration problem in simply supported multi-walled carbon nanotubes (MWCNTs) via the Timoshenko beam model and the generalized shear deformation theory, respectively. In [13], Amin et al. have presented a double elastic beam model for frequency analysis in a double-walled carbon nanotube (DWNT) embedded in an elastic matrix. The analysis has been based on both Euler-Bernoulli and Timoshenko beam theories, for both concentric and non-concentric assumptions considering intertube radial displacements and the related degrees of freedom. Chang and Lee have also employed the Timoshenko beam model, in [14], to study the effects of the flow velocity and the aspect ratio on the vibration frequency of a fluid-conveying SWCNT and the results have been compared with the previous study based on the Euler beam model. An assessment of the Timoshenko beam models has been accomplished by Zhang et al. in [15], where extensive molecular dynamics (MD) simulations have been performed to determine the vibration frequencies of

Received 14 June 2010; accepted 13 April 2011.
Address correspondence to Maria Cinefra, Department of Aeronautic and Space Engineering, Politecnico di Torino, Corso Duca degli Abruzzi 24, Torino, 10129, Italy. E-mail: maria.cinefra@polito.it

SWCNTs with various length-to-diameter ratios, boundary conditions, chiral angles, and initial strain. The results have shown that the Timoshenko beam models, with properly chosen parameters, can be applied to the vibrational analysis of SWCNTs.

However, it is also possible to analyze carbon nanotubes using shell models. In [16], Dong et al. have presented an analytical method to investigate wave propagation in individual MWNTs or MWNTs embedded in an elastic matrix, using a laminated cylindrical shell model. Each of the concentric tubes of the MWNT was an individual elastic shell and is coupled to adjacent tubes through the van der Waals interaction. Foo has adopted a continuum cylindrical shell model for the vibration analysis of SWCNTs [17]. Here, the shell model is based on the Donnell thin shell theory and a comparison with MD solution has shown that both sets of results are, to a certain extent, in agreement. Wang and Zhang [18] have also proposed a two-dimensional elastic shell model to characterize the deformation of single-walled carbon nanotubes and they have concluded that this model can be established with well-defined effective thickness. He et al. have used an elastic multiple shell model for the vibration and buckling analysis of MWCNTs [19, 20]; the effect of the van der Waals (vdW) interaction on the vibration characteristics is considered by introducing a continuum model that accounts for the dependence of vdW interaction coefficients on the change of interlayer spacing and the radii of the tubes. Finally, in [21] a continuum elastic double-shell model, based on von Kàrmàn-Donnell-type non-linear differential equations, has been employed to derive the governing equations of the buckling and post-buckling behavior of DWNTs subjected to a torsional load. Each DWNT tube has been described as an individual elastic shell, which is subject to the vdW interaction between the inner and outer nanotubes.

Among the various problems related to the modeling of CNTs, the present work considers the free vibration response. In order to investigate this topic, Carrera's Unified Formulation (CUF) [22] has been extended to DWNTs. These are assumed as equivalent multilayer cylindrical shells. The Equivalent Single Layer (ESL) and Layer-Wise (LW) approaches, as discussed for classical multilayer structures, are modified to consider the nested tubes of the DWNT as independent and separately vibrating. The vdW interaction between two adjacent tubes can be estimated using the Lennard-Jones model [11] and the assembling procedure of the stiffness matrix is opportunely modified to account for them. The results pertaining to the free vibration problem of double-walled carbon nanotubes are presented and the differences between beam and shell models are emphasized. Particular attention has been paid to vdW interaction, and a comparison has been made between models that take into account the van der Waals forces and models that neglect them.

2. REFINED SHELL THEORIES

In the case of bi-dimensional multi-layered structures (plates and shells), Carrera's Unified Formulation [22] permits a large variety of 2D models to be obtained. These models differ in the order of used expansion in the thickness direction and in the manner the variables are modeled (Equivalent Single Layer (ESL) or Layer Wise (LW) approach). The salient feature of the Unified Formulation is the unified manner in which all the considered variables and fields can be treated. As is usual in shell theories, the considered variables and their variations are split into a set of thickness functions and the relative terms, only depending on in-plane coordinates (α,β). On the basis of this separation, a general variable $\boldsymbol{a}$ and its respective variation $\delta\boldsymbol{a}$ can be written as:

$$\boldsymbol{a}(\alpha,\beta,z) = F_\tau(z)\,\boldsymbol{a}_\tau(\alpha,\beta), \quad \delta\boldsymbol{a}(\alpha,\beta,z) = F_s(z)\,\delta\boldsymbol{a}_s(\alpha,\beta), \quad \text{with} \quad \tau,s = 1,\ldots,N \tag{1}$$

where N is the order of expansion in the thickness direction.

Due to the unified treatment of all the variables, the three displacement components, u_α, u_β, and u_z and their relative variations, can be modeled via Unified Formulation. In the case of ESL models, the expansion of the displacement components is assumed for the whole multi-layer:

$$\begin{aligned}(u_\alpha, u_\beta, u_z) &= F_\tau\,(u_{\alpha\tau}, u_{\beta\tau}, u_{z\tau})\\ (\delta u_\alpha, \delta u_\beta, \delta u_z) &= F_s\,(\delta u_{\alpha s}, \delta u_{\beta s}, \delta u_{zs}),\end{aligned} \tag{2}$$

with Taylor expansions from first up to 4th order: $F_0 = z^0 = 1$, $F_1 = z^1 = z, \ldots, F_N = z^N, \ldots, F_4 = z^4$.

In the case of LW models, each layer k of the given multi-layered structure is separately considered:

$$\begin{aligned}\left(u_\alpha^k, u_\beta^k, u_z^k\right) &= F_\tau^k\,\left(u_{\alpha\tau}^k, u_{\beta\tau}^k, u_{z\tau}^k\right)\\ \left(\delta u_\alpha^k, \delta u_\beta^k, \delta u_z^k\right) &= F_s^k\,\left(\delta u_{\alpha s}^k, \delta u_{\beta s}^k, \delta u_{zs}^k\right),\end{aligned} \tag{3}$$

where combinations of Legendre polynomials are employed as thickness functions:

$$F_t = \frac{P_0 + P_1}{2} \qquad F_b = \frac{P_0 - P_1}{2} \qquad F_l = P_l - P_{l-2} \quad \text{with} \quad \tau,s = t,b,l \quad \text{and} \quad l = 2,3,4. \tag{4}$$

Here, t and b indicate the top and bottom values for each layer, P_l are the Legendre polynomials ($P_0 = 1$, $P_1 = \zeta_k$, $P_2 = \frac{(3\zeta_k^2-1)}{2}$, and so on) with $\zeta_k = \frac{2z^k}{h^k}$ that is the non-dimensionalized thickness coordinate ranging from -1 to $+1$ in each layer k. z_k is the local coordinate and h_k is the thickness of the kth layer.

The chosen functions have the following interesting properties:

$$\begin{aligned}&\zeta_k = +1: \quad F_t = 1; \quad F_b = 0; \quad F_l = 0 \qquad \text{at the top,}\\ &\zeta_k = -1: \quad F_t = 0; \quad F_b = 1; \quad F_l = 0 \qquad \text{at the bottom.}\end{aligned} \tag{5}$$

For further details about CUF for multi-layered structures and the relative assembling procedure of the stiffness matrix, the reader can refer to [22] and [23].

2.1. Governing Equations

This section presents the derivation of the governing equations based on the *Principle of Virtual Displacements* (PVD) in the case of free-vibration analysis of multilayered shells. CUF permits to obtain the so-called *fundamental nuclei*, which are simple matrices representing the basic elements from which the stiffness matrix of the whole structure can be computed. In this part, the van der Walls interaction is not yet considered.

The PVD, for a shell with N_l layers, reads:

$$\int_V \left(\delta\boldsymbol{\epsilon}_{pG}^{kT}\boldsymbol{\sigma}_{pC}^{k} + \delta\boldsymbol{\epsilon}_{nG}^{kT}\boldsymbol{\sigma}_{nC}^{k}\right) dV = \delta L_e^k + \delta L_{in}^k, \tag{6}$$

where Ω_k and A_k are the integration domains in plane (α,β) and z direction, respectively. k indicates the layer and T the transpose of a vector. The stresses and the strains are split in in-plane (p) and normal to the plane (n) components. The first member of the equation represents the variation of internal work δL_{int}^k; δL_e^k is the external work for the kth layer and $\delta L_{in}^k = \int \rho^k \ddot{\boldsymbol{u}}^k \delta\boldsymbol{u}^k dV$ is the virtual inertial work for the kth layer (ρ is the density and $\ddot{\boldsymbol{u}}^k$ denotes the second derivative with respect to the time of the displacement components). G means geometrical relations and C constitutive ones.

The first step to derive the fundamental nuclei is the substitution of *constitutive equations* (C) in the variational statement PVD, which are:

$$\begin{aligned}\boldsymbol{\sigma}_{pC}^{k} &= \boldsymbol{C}_{pp}^{k}\ \boldsymbol{\varepsilon}_{pG}^{k} + \boldsymbol{C}_{pn}^{k}\ \boldsymbol{\varepsilon}_{nG}^{k},\\ \boldsymbol{\sigma}_{nC}^{k} &= \boldsymbol{C}_{np}^{k}\ \boldsymbol{\varepsilon}_{pG}^{k} + \boldsymbol{C}_{nn}^{k}\ \boldsymbol{\varepsilon}_{nG}^{k},\end{aligned} \tag{7}$$

with

$$\boldsymbol{C}_{pp}^{k} = \begin{bmatrix} C_{11} & C_{12} & C_{16} \\ C_{12} & C_{22} & C_{26} \\ C_{16} & C_{26} & C_{66} \end{bmatrix}, \qquad \boldsymbol{C}_{pn}^{k} = \begin{bmatrix} 0 & 0 & C_{13} \\ 0 & 0 & C_{23} \\ 0 & 0 & C_{36} \end{bmatrix},$$

$$\boldsymbol{C}_{np}^{k} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ C_{13} & C_{23} & C_{36} \end{bmatrix}, \qquad \boldsymbol{C}_{nn}^{k} = \begin{bmatrix} C_{55} & C_{45} & 0 \\ C_{45} & C_{44} & 0 \\ 0 & 0 & C_{33} \end{bmatrix}. \tag{8}$$

The second step consists of introducing *geometrical relations*, which relate the strains to the displacement components $\boldsymbol{u} = (u_\alpha, u_\beta, u_z)$. Since, in this work, the multi-walled carbon nanotube is modeled as an equivalent continuum cylindrical shell, the geometrical relations are as follows:

$$\begin{aligned}\boldsymbol{\epsilon}_{pG}^{k} &= [\epsilon_{\alpha\alpha}, \epsilon_{\beta\beta}, \gamma_{\alpha\beta}]^{kT} = \left(\boldsymbol{D}_p^k + \boldsymbol{A}_p^k\right)\ \boldsymbol{u}^k\ ,\\ \boldsymbol{\epsilon}_{nG}^{k} &= [\gamma_{\alpha z}, \gamma_{\beta z}, \epsilon_{zz}]^{kT} = \left(\boldsymbol{D}_{np}^k + \boldsymbol{D}_{nz}^k - \boldsymbol{A}_n^k\right)\ \boldsymbol{u}^k\ ,\end{aligned} \tag{9}$$

wherein the differential operator arrays are defined as follows:

$$\boldsymbol{D}_p^k = \begin{bmatrix} \frac{\partial_\alpha}{H_\alpha^k} & 0 & 0 \\ 0 & \frac{\partial_\beta}{H_\beta^k} & 0 \\ \frac{\partial_\beta}{H_\beta^k} & \frac{\partial_\alpha}{H_\alpha^k} & 0 \end{bmatrix}, \quad \boldsymbol{D}_{np}^k = \begin{bmatrix} 0 & 0 & \frac{\partial_\alpha}{H_\alpha^k} \\ 0 & 0 & \frac{\partial_\beta}{H_\beta^k} \\ 0 & 0 & 0 \end{bmatrix},$$

$$\boldsymbol{D}_{nz}^k = \begin{bmatrix} \partial_z & 0 & 0 \\ 0 & \partial_z & 0 \\ 0 & 0 & \partial_z \end{bmatrix}, \tag{10}$$

$$\boldsymbol{A}_p^k = \begin{bmatrix} 0 & 0 & \frac{1}{H_\alpha^k R_\alpha^k} \\ 0 & 0 & \frac{1}{H_\beta^k R_\beta^k} \\ 0 & 0 & 0 \end{bmatrix}, \quad \boldsymbol{A}_n^k = \begin{bmatrix} \frac{1}{H_\alpha^k R_\alpha^k} & 0 & 0 \\ 0 & \frac{1}{H_\beta^k R_\beta^k} & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{11}$$

For further details about geometrical relations see [23].

By introducing the Unified Formulation for the displacements (Eq. 2), one has:

$$\begin{aligned}\boldsymbol{\epsilon}_{pG}^{k} &= [\epsilon_{\alpha\alpha}, \epsilon_{\beta\beta}, \gamma_{\alpha\beta}]^{kT} = \left(\boldsymbol{D}_p^k + \boldsymbol{A}_p^k\right)\ (F_\tau \boldsymbol{u}_\tau^k),\\ \boldsymbol{\epsilon}_{nG}^{k} &= [\gamma_{\alpha z}, \gamma_{\beta z}, \epsilon_{zz}]^{kT} = \left(\boldsymbol{D}_{np}^k + \boldsymbol{D}_{nz}^k - \boldsymbol{A}_n^k\right)\ (F_\tau \boldsymbol{u}_\tau^k).\end{aligned} \tag{12}$$

After substitutions, the *nucleus* is expanded according to the indicated indexes (τ and s for the order of expansion of primary variables in the thickness direction and k for the multilayer assembling) in order to obtain the matrix for the whole shell.

The governing equation system in the case of PVD is:

$$\delta\boldsymbol{u}_s^{k\,T}\ :\quad \boldsymbol{K}_{uu}^{k\tau s}\,\boldsymbol{u}_\tau^k\ =\ \boldsymbol{P}_{us}^k - \boldsymbol{M}^{k\tau s}\ddot{\boldsymbol{u}}_\tau^k\ , \tag{13}$$

where $\boldsymbol{M}^{k\tau s}$ is the fundamental nucleus for the inertial array, $\boldsymbol{K}_{uu}^{k\tau s}$ is the so-called fundamental nucleus of the stiffness array, and $\boldsymbol{P}_{us}^k$ is the external mechanical load.

The boundary conditions of Neumann type state:

$$\boldsymbol{\Pi}_{uu}^{k\tau s}\,\boldsymbol{u}_\tau^k\ =\ \boldsymbol{\Pi}_{uu}^{k\tau s}\,\bar{\boldsymbol{u}}_\tau^k. \tag{14}$$

For mathematical passages to obtain the governing equations and the explicit form of fundamental nuclei, one can refer to [23].

3. FREE VIBRATION ANALYSIS

Navier-type closed form solutions are applied to the proposed governing equations if the considered materials fulfill the following conditions:

$$C_{16} = C_{26} = C_{36} = C_{45} = 0. \tag{15}$$

The following harmonic assumptions can be made for the field variables:

$$\begin{aligned} u^k_{\alpha_\tau} &= \sum_{m,n} \hat{U}^k_{\alpha_\tau} \cos\frac{m\pi\alpha_k}{a_k} \sin\frac{n\pi\beta_k}{b_k} e^{i\omega_{mn}\hat{t}} \quad k = 1, N_l, \\ u^k_{\beta_\tau} &= \sum_{m,n} \hat{U}^k_{\beta_\tau} \sin\frac{m\pi\alpha_k}{a_k} \cos\frac{n\pi\beta_k}{b_k} e^{i\omega_{mn}\hat{t}} \quad \tau = t, b, r, \\ u^k_{z_\tau} &= \sum_{m,n} \hat{U}^k_{z_\tau} \sin\frac{m\pi\alpha_k}{a_k} \sin\frac{n\pi\beta_k}{b_k} e^{i\omega_{mn}\hat{t}} \quad r = 2, N, \end{aligned} \tag{16}$$

in which a_k and b_k are the shell lengths in the α_k and β_k directions, respectively; m and n are the correspondent wave numbers; $i = \sqrt{-1}$, t is the time, and ω_{mn} is the circular frequency. The quantities with $\hat{}$ indicate the amplitudes. These assumptions correspond to the simply-supported boundary conditions.

The free vibration analysis leads to an eigenvalue problem. Upon substitution of Eqs. (16), the governing equations assume the form of a linear system of algebraic equations in the Ω_k domain:

$$\boldsymbol{K}\hat{\boldsymbol{U}} = \omega^2_{mn}\boldsymbol{M}\hat{\boldsymbol{U}}, \tag{17}$$

where $\boldsymbol{K}$ is the stiffness matrix, $\boldsymbol{M}$ is the inertial matrix, and $\hat{\boldsymbol{U}}$ is the vector of unknown variables. Only the free vibration analysis is investigated in this article, the external mechanical loading is set to zero and the relative boundary conditions are exactly fulfilled. By defining $\lambda_{mn} = \omega^2_{mn}$, the solution of the associated eigenvalue problem becomes:

$$||\boldsymbol{K} - \lambda_{mn}\boldsymbol{M}|| = 0; \tag{18}$$

where $||\ .\ ||$ indicates the determinant of the matrix. The eigenvectors $\hat{\boldsymbol{U}}$ associated to the eigenvalues λ_{mn} (or to circular frequencies ω_{mn}) define the vibration modes of the carbon nanotube in terms of displacements. Once the wave numbers (m,n) have been defined in the in-plane directions, the number of obtained frequencies becomes equal to the degrees of freedom of the employed two-dimensional model.

4. DOUBLE-WALLED CARBON NANOTUBE (DWNT)

It has been demonstrated by Aydogdu [12] that single-beam continuum models, which are often used in literature to study CNTs, cannot represent the behavior of individual tubes in a MWNT and relative deformation between adjacent tubes, because they assume that all the originally concentric tubes of a MWNT remain coaxial during vibration. Therefore, refined MWNTs models are needed, in which also van der Waals (vdW) forces must be taken into consideration and which consider interlayer radial displacements and individual deflection curves of nested tubes within the MWNT.

In this work, the discrete DWNT is considered as an equivalent continuum cylindrical shell composed of two adjacent layers (see Figure 1). As multi-beam models, CUF permits to consider each tube of the DWNT as independent by simply modifying the assembling procedure of the stiffness matrix on the layer k, as shown in Figure 2. In this way, the condition

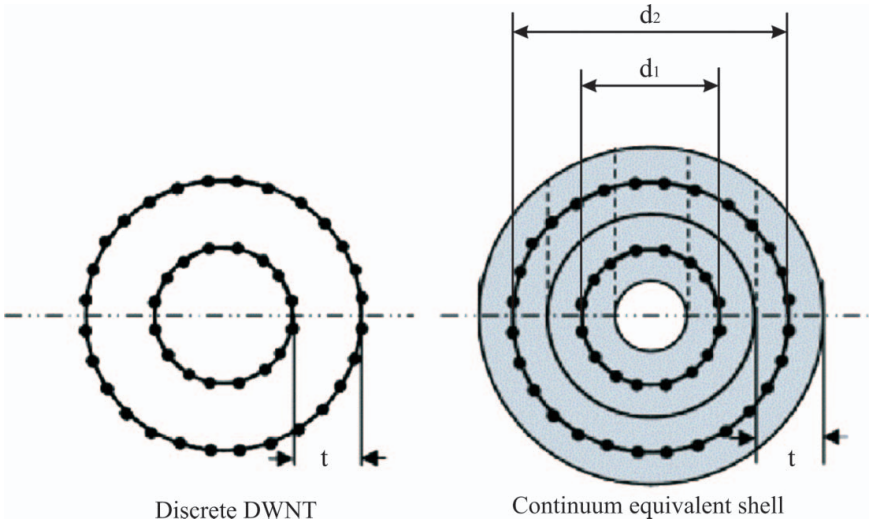

FIG. 1. DWNT: continuum equivalent shell (Color figure available online).

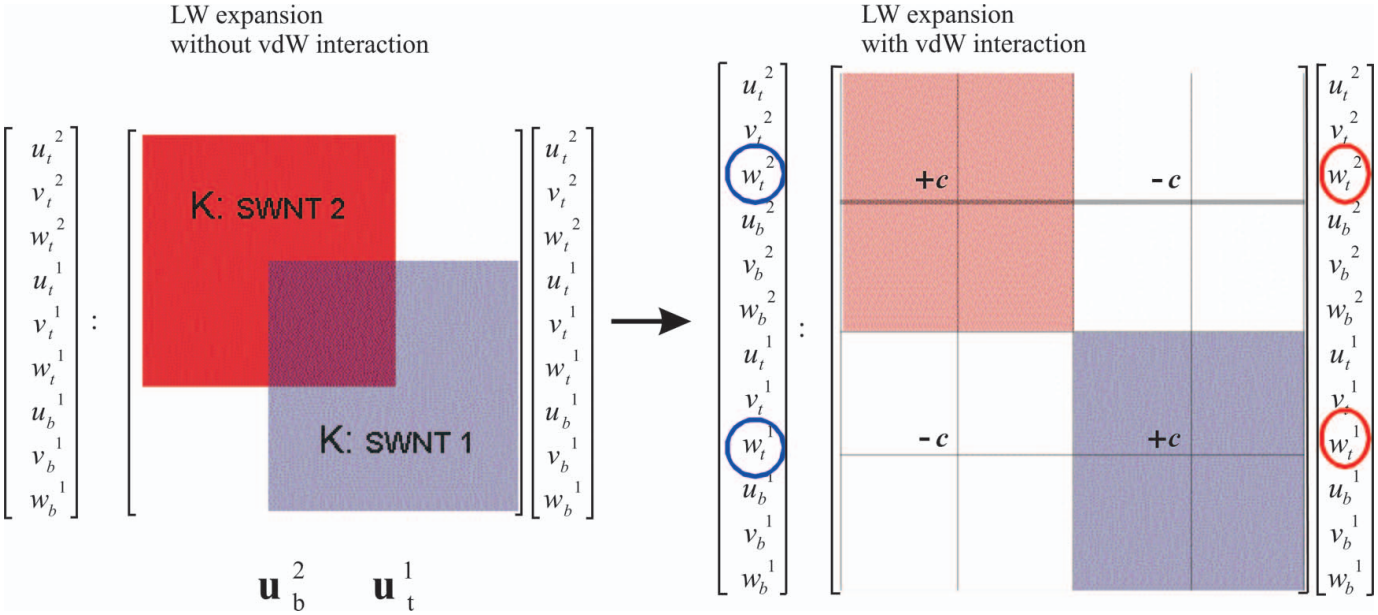

FIG. 2. Assembling procedure of the global stiffness matrix of a DWNT, taking account for van der Waals interaction (Color figure available online).

of continuity for the displacements at the layer interface is not fulfilled and the inner and outer tubes can vibrate separately.

In order to apply a continuum model for the free vibration, analysis of the DWNT is necessary to determine its equivalent mechanical properties. In the literature, there are many dissenting opinions about the mechanical characterization of carbon nanotubes. This work is directed to validate the refined shell theories contained in CUF for the analysis of DWNTs. According to [12], the effective wall thickness of the single carbon nanotube t is assumed to be equal to the interplanar spacing of graphite layers (0.35 nm) and the mechanical properties are consequently calculated. The diameters of the inner and the outer walls of the double-walled nanotube are taken as $d_1 = 0.7$ nm and $d_2 = 1.4$ nm, respectively (see Figure 1). Young's modulus and the shear modulus of double-walled carbon nanotubes are assumed to be approximately insensitive to tube chirality. For the present DWNT and tube geometry, each tube is assumed to have the same Young's modulus of 1 TPa, shear modulus of 0.4 TPa, Poisson ratio of 0.25, and mass density of 2.3 g/cm^3 with the effective thickness of 0.35 nm.

The deflections of two tubes are coupled through the van der Waals intertube interaction pressure. Since the inner and outer tubes of a DWNT are originally concentric and the van der Waals interaction is determined by the interlayer spacing, the net van der Waals interaction pressure remains zero for each tube, provided they deform coaxially. For small-amplitude linear transverse vibrations, interaction pressure at any point between the tubes depends linearly on the difference between their deflection curves at that point. The van der Waals pressure on tube 1 due to tube 2 (see Figure 3), which is positive inward, is given in [12]:

$$P_{1,2} = c(w_2 - w_1), \tag{19}$$

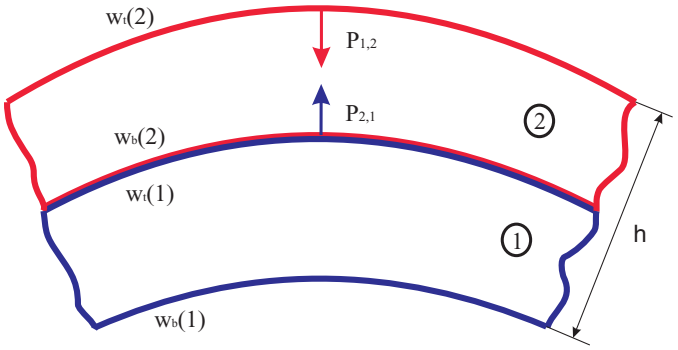

FIG. 3. van der Waals interaction in a DWNT (Color figure available online).

and, for the equilibrium, $P_{2,1} = -P_{1,2}$. w_1 and w_2 are the displacements of the tubes in the radial direction and c is the van der Waals interaction coefficient, estimated at the initial interlayer spacing (~ 0.34 nm):

$$c = \frac{320 \text{ erg/cm}^2}{0.16 d^2}, \tag{20}$$

where $d = 0.142$ nm is the length of C-C bond and 1 erg $= 10^{-7}$ J.

Since the coefficient c has the physical dimensions of a stiffness, it is possible to account for vdW interaction in the CUF by

TABLE 1
Natural frequencies parameter Ω of DWNT. STOB results are provided in [12]. $L/h = 10$ and $m = 2$

n	STOB	CLT	FSDT	$ED1$	$ED2$	$ED3$	$ED4$
1	3.1278	3.1278	3.1254	3.1310	3.1220	3.1219	3.1219
2	6.1735	6.1604	6.1422	6.1538	6.1356	6.1345	6.1344
3	9.0418	9.0283	8.9772	8.9955	8.9675	8.9644	8.9641
4	11.612	11.704	11.601	11.627	11.589	11.582	11.582
5	13.757	14.190	14.016	14.050	14.001	13.991	13.989

TABLE 2
Natural frequencies parameter Ω of DWNT. STOB results are provided in [12]. $L/h = 50$ and $m = 2$

n	STOB	CLT	FSDT	$ED1$	$ED2$	$ED3$	$ED4$
1	3.1410	3.1455	3.1442	3.1497	3.1408	3.1408	3.1408
2	6.2787	6.2867	6.2835	6.2947	6.2768	6.2768	6.2768
3	9.4102	9.4194	9.4135	9.4302	9.4034	9.4032	9.4032
4	12.531	12.540	12.529	12.552	12.516	12.516	12.515
5	15.640	15.644	15.627	15.655	15.610	15.609	15.609

TABLE 3
Natural frequencies parameter Ω of DWNT. DTOB results are provided in [12]. vdW forces are taken into consideration. $L/h = 10$ and $m = 2$

n	DTOB	$LD1$	$LD2$	$LD3$	$LD4$
1	3.1199	3.1155	3.1135	3.1135	3.1135
2	6.1275	6.0776	6.0733	6.0732	6.0732
3	8.9633	8.7914	8.7866	8.7841	8.7841
4	11.547	11.230	11.220	11.219	11.219
5	13.761	13.410	13.386	13.395	13.395

TABLE 4
Natural frequencies parameter Ω of DWNT. DTOB results are provided in [12]. vdW forces are taken into consideration. $L/h = 50$ and $m = 2$

n	DTOB	$LD1$	$LD2$	$LD3$	$LD4$
1	3.1406	3.1425	3.1404	3.1404	3.1404
2	6.2760	6.2781	6.2740	6.2740	6.2740
3	9.4008	9.4000	9.3939	9.3939	9.3939
4	12.510	12.502	12.494	12.494	12.494
5	15.599	15.578	15.567	15.567	15.567

TABLE 5
Natural frequencies parameter Ω of DWNT. Comparison between ESL models and LW models which account for vdW forces: $\Delta(\%) = \frac{ED4-LD4}{ED4} \times 100$

	$L/h = 10$			$L/h = 50$		
n	$ED4$	$LD4$ (vdW)	$\Delta(\%)$	$ED4$	$LD4$ (vdW)	$\Delta(\%)$
1	3.1219	3.1135	0.27	3.1408	3.1404	0.01
2	6.1344	6.0732	1.00	6.2768	6.2740	0.04
3	8.9641	8.7841	2.00	9.4032	9.3939	0.10
4	11.582	11.219	3.13	12.515	12.494	0.17
5	13.989	13.395	4.25	15.609	15.567	0.27

opportunely introducing c in the stiffness matrix, as shown in Figure 2. This is equivalent to considering the van der Waals forces $P_{2,1}$ and $P_{1,2}$ as external loads applied at the top of the layers 1 and 2, respectively.

5. RESULTS AND DISCUSSION

In this section, the results obtained using the CUF extended to free vibrations analysis of the double-walled carbon nanotube, presented in the previous section, are proposed. The global thickness of DWNT is $h = 1.75$ and the thickness ratio L/h, where L is the axial length of the nanotube, assumes the values 10 and 50.

In Tables 1 and 2, the tubes of DWNT are supposed to remain coaxial during vibration, while in Tables 3 and 4, each tube of DWNT is considered as independent and the vdW interaction is accounted for. These results are compared with the beam solutions provided in [12], by Aydogdu: Tables 1 and 2 refer to the single third-order beam (STOB) theory and Tables 3 and 4 to the double third-order beam (DTOB) theory. The proposed values are calculated employing different two-dimensional shell models contained in the CUF: Classical Lamination Theory (CLT), First order Shear Deformation Theory (FSDT), Equivalent Single Layer and Layer Wise models with order of expansion for the displacements in the thickness direction from 1 to 4, these are $ED1 - ED4$ and $LD1 - LD4$ models, respectively.

In the tables, the wave numbers of the vibration modal shapes of DWNT in terms of displacements, in the axial and circumferential directions, are taken as $n = 1, ..., 5$ and $m = 2$, respectively. Only first-order frequencies are considered and these are normalized according to the formula:

$$\Omega = \sqrt[4]{\frac{\rho A \omega^2 L^4}{EI}}, \tag{21}$$

where A and I are the area and moment of inertia of the DWNT cross section.

Tables 1–4 show that the CUF results are in good agreement with the reference solution by increasing the order of expansion of the theory. It should be considered that shell models are compared with beam models, therefore, some differences between them remain even though high orders of expansion ($N = 4$) are used. However, these differences become smaller when the nanotube is longer ($L/h = 50$), because the beam hypotheses are fulfilled, and lower frequencies are considered (low n). In particular, looking at Tables 1 and 2 it is possible to note that in general CLT and FSDT theories give results that are further from the reference solution, compared with the ESL models. In some cases, such as in Table 2 for $n = 4$ and $n = 5$, CLT and FSDT theories give a smaller error in respect to high-order equivalent single layer theories, but this inconsistency is due to the error that a beam model, as is the STOB, produces on high frequencies. $ED4$ and $LD4$ models are compared in Table 5. The percentage difference $\Delta(\%) = \frac{ED4-LD4}{ED4} \times 100$ between them increases for short DWNTs and higher frequencies, therefore, it is possible to conclude that in these cases it is necessary to consider the vdW interaction between the DWNT tubes in order to avoid overestimated results.

6. CONCLUSIONS

This work has applied refined shell models, by extending the Unified Formulation, to study the dynamic response of double-walled carbon nanotubes. The DWNT is assumed to be an equivalent continuum cylindrical shell made up of two layers and both ESL and LW models have been employed in the analysis. LW models have been modified in order to consider two DWNT tubes as separately vibrating and to account for the van der Waals interaction between them. The following conclusions can be drawn:

- Refined shell models can successfully be extended to the free vibration analysis of DWNTs and they give a satisfactory analysis for both long and short CNTs, for both lower and higher frequencies.
- The introduction of the van der Waals forces makes it possible to consider two adjacent tubes and leads to lower frequency values.
- The introduction of the vdW forces is mandatory for short CNTs and/or higher frequencies.

The authors are aware of the limitations of continuum mechanics models. Future work will be performed to couple molecular dynamic analysis to the present refined shell models.

ACKNOWLEDGMENTS

The authors acknowledge the partial support of the Piemonte Regional Project STEPS. M Cinefra acknowledges the support of FNR, Luxembourg.

REFERENCES

1. S. Iijima, Helical microtubules of graphitic carbon, Nature, vol. 354, pp. 56–58, 1991.
2. A. Sakhaee-Pour, M.T. Ahmadian, and A. Vafai, Vibrational analysis of single-walled carbon nanotubes using beam element, Thin-Walled Struct., vol. 47, pp. 646–652, 2009.
3. M. Mir, A. Hosseini, and G.H. Majzoobi, A numerical study of vibrational properties of single-walled carbon nanotubes, Comput. Mater. Sci., vol. 43, pp. 540–548, 2008.
4. G.M. Odegard, T.S. Gates, L.M. Nicholson, and K.E. Wise, Equivalent-continuum modeling of nanostructured materials, Compos. Sci. Technol., vol. 62, no. 14, pp. 1869–1880, 2002.
5. T. Vodenitcharova and L.C. Zhang, Effective wall thickness of a single-walled carbon nanotube, Phys. Rev. B, vol. 68, p. 165401, 2003.
6. G. Rouainia and K. Djeghaba, Evaluation of Young's modulus of single walled carbon nanotube (SWNT) reinforced concrete composite, J. Eng. Appl. Sci., vol. 3, no. 6, pp. 504–515, 2008.
7. C.Y. Wang and L.C. Zhang, A critical assessment of the elastic properties and effective wall thickness of single-walled carbon nanotubes, Nanotechnology, vol. 19, p. 075705, 2008.

8. Y.D. Kuang and X.Q. He, Young's moduli of functionalized single-wall carbon nanotubes under tensile loading, Compos. Sci. Tech., vol. 69, pp. 169–175, 2009.
9. L.C. Zhang, On the mechanics of single-walled carbon nanotubes, J. Mater. Process. Tech., vol. 209, pp. 4223–4228, 2009.
10. C.M. Wang, V.B.C. Tan, and Y.Y. Zhang, Timoshenko beam model for vibration analysis of multiwalled carbon nanotubes, J. Sound Vibra., vol. 294, pp. 1060–1072, 2006.
11. M. Aydogdu, Vibration of multi-walled carbon nanotubes by generalized shear deformation theory, Int. J. Mech. Sci., vol. 50, pp. 837–844, 2008.
12. M. Aydogdu, Effects of shear deformation on vibration of doublewalled carbon nanotubes embedded in an elastic medium, Arch. Appl. Mech., vol. 78, pp. 711–723, 2008.
13. S.S. Amin, H. Dalir, and A. Farshidianfar, Carbon nanotube-reinforced composites: Frequency analysis theories based on the matrix stiffness, Comput. Mech., vol. 43, pp. 515–524, 2009.
14. W.J. Chang and H.L. Lee, Free vibration of a single-walled carbon nanotube containing a fluid flow using the Timoshenko beam model, Phys. Lett. A, vol. 373, pp. 982–985, 2009.
15. Y.Y. Zhang, C.M. Wang, and V.B.C. Tan, Assessment of Timoshenko beam models for vibrational behavior of single-walled carbon nanotubes using Molecular Dynamics, Adv. Appl. Math. Mech., vol. 1, no. 1, pp. 89–106, 2009.
16. K. Dong, S.Q. Zhu, and X. Wang, Wave propagation in multiwall carbon nanotubes embedded in a matrix material, Compos. Struct., vol. 82, pp. 1–9, 2008.
17. C.N. Foo, Vibration of single-walled carbon nanotubes based on cylindrical shell model, http://www.nus.edu.sg/nurop/2009/FoE/U076369B.PDF
18. C.Y. Wang and L.C. Zhang, An elastic shell model for characterizing single-walled carbon nanotubes, Nanotechnology, vol. 19, p. 195704, 2008.
19. X.Q. He, M. Eisenberger, and K.M. Liew, The effect of van der Waals interaction modeling on the vibration characteristics of multiwalled carbon nanotubes, J. Appl. Phys., vol. 100, pp. 1–12, 2006.
20. X.Q. He, S. Kitipornchai, and K.M. Liew, Buckling analysis of multi-walled carbon nanotubes: A continuum model accounting for van der Waals interaction, J. Mech. Phys. Solids, vol. 53, pp. 303–326, 2005.
21. X. Yao and Q. Han, Torsional buckling and postbuckling equilibrium path of double-walled carbon nanotubes, Compos. Sci. Tech., vol. 68, pp. 113–120, 2008.
22. E. Carrera, A class of two dimensional theories for multilayered plates analysis, Atti Accademia delle Scienze di Torino, Mem. Sci. Fis., vol. 19–20, no. 49–87, 1995.
23. E. Carrera, Theories and finite elements for multilayered plates and shells: A unified compact formulation with numerical assessment and benchmarking, Arch. Comput. Meth. Engineer., vol. 10, pp. 215–297, 2003.