Vibrations analysis of multiwalled carbon nanotubes by refined shell theories

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Abstract

Much research has been carried out on carbon nanotubes (CNTs) since their discovery in Japan by Ijima [1] in 1991. Carbon nanotubes exhibit superior mechanical properties and hold substantial promise by providing strong, light, and high toughness characteristics. CNTs are theoretically assumed to be made by rolling a graphene sheet about an opportune vector $\overrightarrow{T}$. A chiral vector $\overrightarrow{C}_h$, perpendicular to the vector $\overrightarrow{T}$, can be defined. The chiral vector is expressed in terms of base vectors $\overrightarrow{a}_1$ and $\overrightarrow{a}_2$ as:

$$\overrightarrow{C}_h = n\overrightarrow{a}_1 + m\overrightarrow{a}_2 \tag{1}$$

where n and m are lattice translational indices. If the chiral vector is described by $(n, 0)$ or (m, m) indices, the structure is zigzag or armchair, respectively [2].

There are two basic methods in simulating mechanical behavior of the nanostructures: atomistic-based modelling approaches and continuum ones. In the former, the vibrational behavior of CNTs is investigated by using an atomistic finite element model with beam elements and concentrated masses [2]. The beams simulate the interatomic covalent forces and the masses are located at the ends of the beams representing the carbon position: the computational effort for these methods does not permit simulation of real size multi-walled CNTs. For these reasons, continuum approaches are preferred to atomistic-based models. Among the various problem related to the modelling of CNTs, the present work considers the free vibrations response. Wang [3] and Aydogdu [4] studied vibrations problem in simple supported multi-walled carbon nanotubes (MWCNTs) via beam models (Timoshenko and Parabolic Shear Deformation Theory (PSDT)). He et alii used an elastic multiple shell model for the vibration and buckling analysis of MWCNTs [5], [6]; the effect of van der Waals (vdW) interaction on the vibration characteristics is considered by introducing a continuum model accounting for the dependence of vdW interaction coefficients on the change of interlayer spacing and the radii of tubes.

In order to investigate the free vibrations of MWCNTs, Carrera's Unified Formulation (CUF) [7] is extended in this work. MWCNTs are assumed as a multilayer cylindrical shell. The displacement components $\boldsymbol{u}$, as well as their virtual variations $\delta\boldsymbol{u}$, are modelled in the thickness direction z as:

$$\delta\boldsymbol{u}(\alpha, \beta, z) = F_\tau(z)\delta\boldsymbol{u}_\tau(\alpha, \beta)\ , \qquad \boldsymbol{u}(\alpha, \beta, z) = F_s(z)\boldsymbol{u}_s(\alpha, \beta) \tag{2}$$

where F_τ and F_s are the thickness functions, (α, β, z) is the orthogonal curvilinear reference system for a shell geometry, $\boldsymbol{u} = (u, v, w)$ is the vector containing the three displacements components.

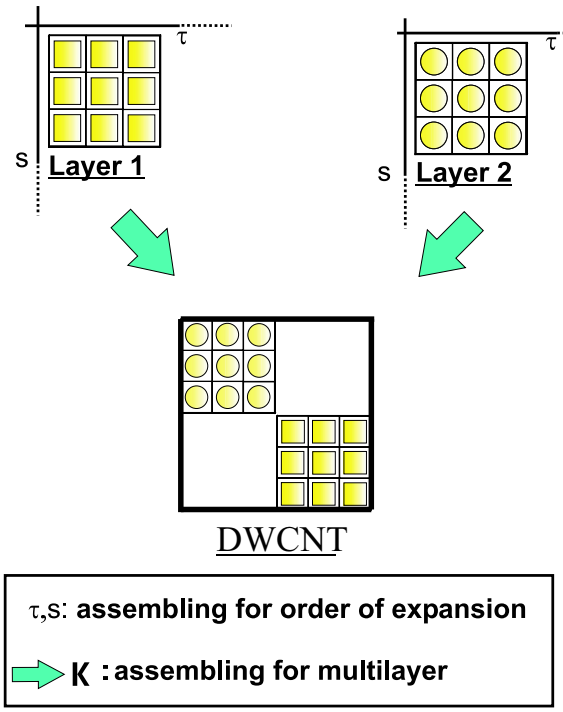

Figure 1: Example of assembling procedure for a MWCNT.

The related governing equations in the dynamic case of free vibrations are:

$$\delta \boldsymbol{u}_\tau : \quad \boldsymbol{K}^{k\tau s}\boldsymbol{u}_s = \boldsymbol{M}^{k\tau s}\ddot{\boldsymbol{u}}_s \tag{3}$$

where $\boldsymbol{K}^{k\tau s}$ and $\boldsymbol{M}^{k\tau s}$ are the so-called fundamental nuclei. The stiffness and the inertial matrix of the considered MWCNT are obtained by assembling via the indices k, τ, s as indicated in Fig. 1.

Equivalent Single Layer (ESL) and Layer-Wise (LW) approaches, as discussed for classical multilayer structures, are modified to consider nested tubes of a MWCNT as independent and separately vibrating. The vdW interaction potential between two adjacent tubes can be estimated using the Lennard-Jones model [4]. For small-amplitude linear transverse vibrations, interaction pressure p at any point between the tubes should be a linear function of the deflection jump at that point:

$$p = c(w_2 - w_1) \tag{4}$$

where c is the estimated vdW interaction coefficient, w_1 and w_2 are the transverse displacements of layer 1 and 2, respectively. The pressure p may be seen as an external load that reduces the stiffness of layer 2 and increases that of layer 1 (see Fig. 1). The Eq.(4) rewritten for a generic MWCNT is:

$$p_i = c_i(w_N - w_{N-1}) \tag{5}$$

where i is the considered inter-layer. $N = 1, ..., N_l$ indicates the number of layers.

Results for the free vibrations problem of single-walled, double-walled and multi-walled carbon nanotubes will be presented at the conference. Differences between beam and shell models will be emphasized. Particular attention will be devoted to van der Waals (vdW) interaction, by comparing models accounting for vdW

forces with those without vdW forces.

References

[1] S. Ijiam, *"Helical microtubules of graphitic carbon"*, Nature, 354, 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 Structures, in press, available on line 20 January 2009.

[3] C.M. Wang, V.B.C. Tan and Y.Y. Zhang, *"Timoshenko beam model for vibration analysis of multiwalled carbon nanotubes"*, Journal of Sound and Vibration, 294, 1060-1072, 2006.

[4] M. Aydogdu, *"Vibration of multi-walled carbon nanotubes by generalized shear deformation theory"*, International Journal of Mechanical Sciences, 50, 837-844, 2008.

[5] 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"*, Journal of Applied Physics, 100, 1-12, 2006.

[6] 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"*, Journal of Mechanics and Physics of solids, 53, 303-326, 2005.

[7] E. Carrera, *"A class of two dimensional theories for multilayered plates analysis"*, Atti Accademia delle Scienze di Torino, Mem Sci. Fis., 19-20, 49-87, 1995.