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Flexural Dynamic Properties of Single-Walled Carbon Nanotube and Carbon-Nanotube-Reinforced-Polymer

Jorge Alberto Palacios, Rajamohan Ganesan
Department of Mechanical, Industrial and Aerospace Engineering, Concordia University
1455 de Maisonneuve Blvd. West, Montreal, Que., Canada H3G 1M8
j_palaci@live.concordia.ca; r.ganesan@concordia.ca

Abstract – During last few decades the application of carbon nanotubes as an option of reinforcing element in nanocomposites, has become considerably popular, particularly in the aerospace and aeronautical industry. Nanocomposites are preferred over conventional materials because of their superior mechanical properties, such as high specific strength, high stiffness, low density and fatigue resistance. However, studies still need to be carried out, especially for dynamic response of the nanostructure and the reinforcement in the composite. Therefore, the objective of this work is to model a Single-Walled Carbon Nanotube (SWCN) as a space frame structure by using the modified Morse potential and as a thin shell based on Donnell's theory to analyze its dynamic properties, in terms of its natural frequencies, under different types of boundaries conditions, and a Carbon-Nanotube-Reinforced-Polymer (CNRP) by developing a 3D multiscale finite-element model of the composite under the same boundary conditions. The natural frequencies of the SWCN obtained from the modified Morse potential are compared with the natural frequencies obtained from the shell theory, while the natural frequencies of the CNRP are compared with the natural frequencies of the polymer.

***Keywords*:** Carbon-Nanotube-Reinforced-Polymer, Multiscale Modeling, Finite Element Analysis, Natural Frequencies, Natural Modes, Thin Shell.

1. Introduction

Carbon nanotubes, reported first time by Iijima [1] in 1991, have attracted great attention worldwide because of their excellent properties, such as extremely high stiffness and strength. They have been widely considered as a great potential to be used as reinforcing elements in advanced composite materials in a large number of engineering applications. Therefore, the purpose of this research is to conduct a design parametric study to analyze the dynamical response of a Single-Walled Carbon Nanotube (SWCN) modeled as a space frame structure by using the modified Morse potential and as a thin shell under different types of boundary conditions; and a Carbon-Nanotube-Reinforced-Polymer (CNRP) by developing and using a 3D multiscale finite-element model of the Representative Volume Element (RVE) of the composite under the same boundary conditions. The RVE investigated in this work consists of a single-walled carbon nanotube (SWCN) embedded in a polymer matrix and an interface region between the SWCN and the polymer material. The polymer matrix is modeled with the Mooney-Rivlin strain energy to calculate its non-linear response and the interface region is modeled via van der Waals (vdW) links based the Lennard-Jones Potential.

2. Methodology for Finite Element Modelling of Composite

The volume fraction of the SWCN in the composite with respect to the proposed RVE can be calculated as follows [2]:

$$V_n = \frac{8r_n t_n}{4r_m^2 - (2r_n - t_n)^2} \tag{1}$$

where r_n is the mean radius of the nanotube, r_m is the radius of the matrix material and t_n is the thickness of the nanotube. The matrix is regarded as a continuum medium since the matrix volume is greater than the SWCN for the volume fractions considered. In order to describe the mechanical behaviour of the polymer matrix, the Mooney–Rivlin strain energy density function is utilized and described as follows [3]:

$$W(I_1, I_2, I_3, v_m) = c_{1m}(I_1 - 3) + c_{2m}(I_2 - 3) + +c_{3m}(I_1 - 3)(I_2 - 3) + \frac{1}{2}k_m(I_3 - 3)^2 \tag{2}$$

where I_1, I_2, and I_3 define the invariants of the strain tensor, v_m is the Poisson's ratio, c_{1m} , c_{2m} and c_{3m} are material parameters and k_m is the bulk modulus of the material. A polyetheretherketone (PEEK) matrix [4] is used as the polymer material with the Mooney-Rivlin parameters: c_{1m}= -3.75 GPa, c_{2m}= 4.82 GPa and c_{3m}= 1.5 GPa. The Young's modulus E_m can be obtained from the stress-strain nonlinear analysis in order to perform the vibration analysis. Therefore, the mechanical properties of a natural rubber used in the vibration analysis are as follows: E_m= 4.9 x 10^9 Pa, density ρ_m = 1.3 x 10^3 kg/m^3, radius r_m = 3.7 nm and Poisson's ratio v_m= 0.3. The bulk modulus k_m is taken to be 4.083 x 10^9 Pa.

Non-linear mechanical behaviour of a SWCN is based on its atomistic nanostructure and is developed around its mean radius r_n. The nanotube modeled is a (20, 0) SWCN with a radius equal to r_n= 0.7834 nm and thickness t_n= 0.34 nm. The nanotube is modeled as a space frame structure where carbon atoms are represented by nodes and covalent bonds as non-linear beam elements to represent the potential energy of the interatomic interactions, which is expressed by the Morse potential. The force stretching $F_{stretch}$ of the non-linear behaviour of these beams can be obtained as follows [2]:

$$F_{stretch}(\Delta r) = 2\beta D_e\left(1 - e^{-\beta\Delta r}\right)e^{-\beta\Delta r} \tag{3}$$

where $\Delta r = r - r_0$ is the bond length variation, and the force parameters are: D_e = 6.03105 x 10^{-19} Nm, β = 2.625 x 10^{10} m^{-1} and r_0 = 1.421 x 10^{-10} m. Although the stress-strain curve and the Young's modulus E_n can be obtained from the previous analysis to perform a vibration analysis, the modified Morse potential can be used to perform a free vibration and harmonic analysis by considering the numerical values for the density ρ_B = 2.3 x 10^3 kg/m^3 for the beams and the mass of the carbon atom = 2.0 x 10^{-26} kg. However, to save a great deal of time and computing efforts, and to study other mechanical properties, such as bending, buckling and torsion, the molecular model can be replaced with a thin shell based on Donnell's shell theory [5] constructed from nonlinear elements in the shape of a hollow cylinder. The nanostructures can be modeled using a shell theory by assuming v_n = 0.19 and t_n = 0.066 nm. [6], including nonlinear effects from the stress-strain curves of the nanotube and the density ρ_n = 1.319 x 10^3 kg/m^3 for the nanotube. The effective transversal area for the thin shell is calculated with the diameter D = 1.5668 nm of the nanotube and the new thickness, which is expressed by $\pi D t_n/(1 - v_n^2)$.

From the structural point of view, the interface can be simulated either as a continuum or as a discrete region. In discrete modeling of the interface, the SWCN can be simulated as a discrete structure by using beam/spring elements, however in this work the SWCN is simulated as a shell structure, while the polymer is modeled by solid elements. The interface region is constructed with the use of truss/spring elements connecting carbon atoms of the discrete structure of SWCN to nodes of the inner surface of matrix elements. The properties of the link elements are obtained by using the corresponding van der Waals forces based on the Lennard-Jones potential as follows [7]:

$$F_{vdW}(r) = -\frac{dU(r)}{dr} = 24\frac{\varepsilon}{\sigma}\left[2\left(\frac{\sigma}{r}\right)^{13} - \left(\frac{\sigma}{r}\right)^{7}\right] \tag{4}$$

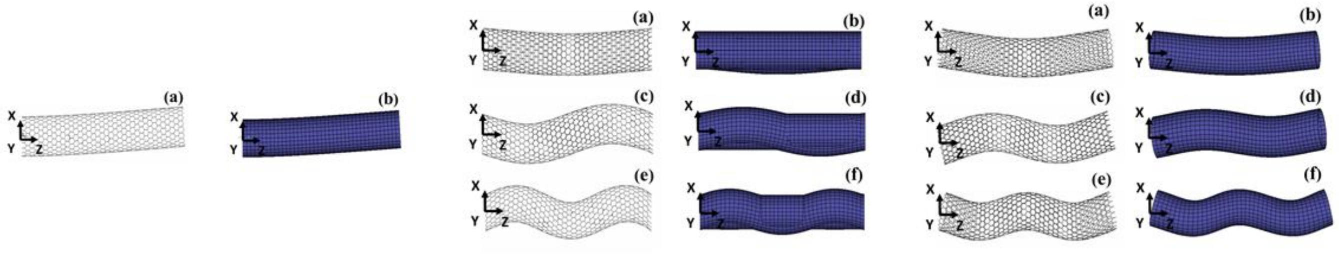
where, r is the distance between interacting atoms, ε and σ are the Lennard–Jones parameters. For carbon atoms, the Lennard–Jones parameters are ε = 0.0556 kcal/mole and σ = 0.34 nm. For simulations of van der Waals interactions at the nanotube/polymer interface, a truss rod model, which was introduced by [7], is adopted.

3. Results and Discussion

The natural frequencies of a (20, 0) SWCN (with length $L_n = 7.96$ nm) are obtained, from the modified Morse potential and the thin shell, and reported in Table 1 for the boundary conditions: Clamped-Free, Clamped-Clamped and Free-Free. The mode shapes with both models are depicted in Fig. 1, which shows a good agreement between the results obtained with the Morse potential and the thin shell based on Donnell's shell theory, as well as sufficient accuracy of SWCN modeling.

Table 1: Natural frequencies (GHz) of a (20, 0) SWCN with different boundary conditions.

Clamped-Free			**Clamped-Clamped**			**Free-Free**		
Mode	**Morse Potential**	**Thin shell**	**Mode**	**Morse Potential**	**Thin shell**	**Mode**	**Morse Potential**	**Thin shell**
First bending	1.504	1.504	First deflection	6.726	6.504	First deflection	8.402	8.381
			Second deflection	14.19	14.13	Second deflection	17.91	18.85
			Third deflection	22.74	22.45	Third deflection	27.62	27.93



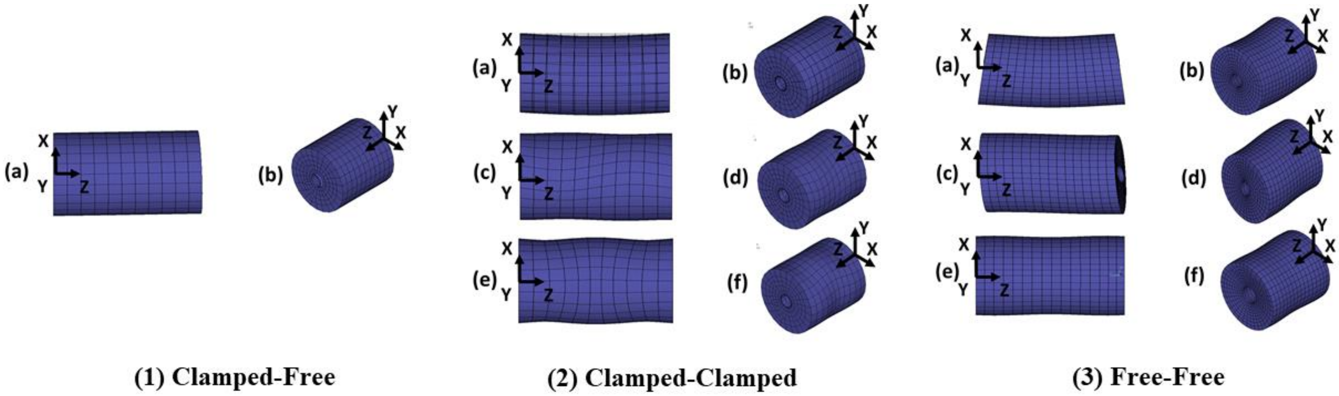
(1) Clamped-Free **(2) Clamped-Clamped** **(3) Free-Free**

Fig. 1: Mode shapes of a (20,0) SWCN with different boundaries conditions: (1) Clamped-Free. (2) Clamped-Clamped and (3) Free-Free. Morse potential is located on the left side and the thin shell on the right side.

The CNRP is analyzed for a 0.04% of volume fraction (V_n), according to the dimensions of the RVE with a length $L_n = 7.96$ nm. Boundary conditions are applied to the 3D multiscale finite-element model just in the polymer matrix, so that the SWCN can transfer its mechanical properties into the matrix through the vdW links. Fig. 2 shows the shapes for the CNRP and the polymer under different boundary conditions, while the natural frequencies obtained for both models are compared in Table 2. As it can be appreciated, the natural frequencies of RVE are higher than those of the polymer model. This can be attributed to the high stiffness and strength of the CNRP due to reinforcement with SWCN. In the CNRP, the SCWN transfers its mechanical properties into the polymer matrix via vdW links, so that the mechanical properties of the composite material improve and its natural frequencies increase.

Table 2: Natural frequencies (GHz) of CNRP with different boundary conditions.

Clamped-Free			**Clamped-Clamped**			**Free-Free**		
Mode	**CNRP**	**Polymer**	**Mode**	**CNRP**	**Polymer**	**Mode**	**CNRP**	**Polymer**
First bending	0.319	0.233	First deflection	0.677	0.67	First deflection	1.022	0.944
			Second deflection	2.145	1.524	Second deflection	1.486	1.04
			Third deflection	2.196	2.094	Third deflection	1.994	1.787



(1) Clamped-Free **(2) Clamped-Clamped** **(3) Free-Free**

Fig. 2: Mode shapes of RVE of the composite with different boundaries conditions: (1) Clamped-Free; (a)-(b) first bending. (2) Clamped-Clamped; (a)-(b) first, (c)-(d) second, and (e)-(f) third deflection shape. (3) Free-Free; (a)-(b) first, (c)-(d) second, and (e)-(f) third deflection shape.

4. Conclusion

The shell model developed in the present work shows sufficient accuracy of SWCN modeling and it can be used to study other mechanical properties, such as buckling and torsion response in addition to flexural response. The results of the calculations of the natural frequencies present a percentage of error in the range of 1.1 - 13% for the 3 types of boundary conditions. This error can be attributed to the non-linear mechanical behavior of SWCN or to the parameters of the thin shell based that were obtained based on Donnell's shell theory. Regarding the CNRP, the results show an increase in the natural frequencies of the composite due to reinforcement with the SWCN, where the first bending mode frequency increases by 36% for the Clamped-Free boundary condition; while for the Clamped-Clamped condition, the first deformation shape amplitude increases by 1%, the second deformation shape amplitude by 40% and the third deformation shape amplitude by 4.8%. Regarding the last boundary condition for the composite, Free-Free, the first deformation shape amplitude increases by 8.2%, the second one by 42% and the third one by 11.5%.

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References

[1] S. Iijima, "Helical microtubules of graphitic carbon," *Nature*, vol. 354, no. 568, pp. 56-58, 1991.

[2] S. Georgantzinos, G. Giannopoulos, and N. Anifantis, "Investigation of stress–strain behavior of single walled carbon nanotube/rubber composites by a multi-scale finite element method," *Theoretical and Applied Fracture Mechanics*, vol. 52, no. 3, pp. 158-164, 2009.

[3] R. W. Ogden, *Non-Linear Elastic Deformations*. Dover Publications, 1997.

[4] Z. El-Qoubaa, and R. Othman, "Characterization and modeling of the strain rate sensitivity of polyetheretherketone's compressive yield stress," *Materials and Design*, vol. 66, pp. 336-345, 2015.

[5] L. H. Donnell, *Beams, Plates and Shells*. New York: McGraw-Hill Book Company, 1976.

[6] B. I. Yakobson, C. J. Brabec, and J. Bernholc, "Nanomechanics of Carbon Tubes: Instabilities Beyond Linear Response," *Physical Review Letters*, vol. 76 no. 14, pp. 2511-2514. 1996.

[7] J. M. Wernik, B. J. Cornwell-Mott, and S. A. Meguid, "Determination of the Interfacial Properties of Carbon Nanotube Reinforced Polymer Composites using Atomistic-Based Continuum Model," *International Journal of Solids and Structures*, vol. 49, no. 13, pp. 1852-1863, 2012.