Buckling Behavior of 3D Randomly Oriented CNT Reinforced Nanocomposite Plate

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Abstract: In this paper, the influence of carbon nanotube (CNT) in a metal matrix on the buckling behavior of the resulting nanocomposite plate is studied. The Young's modulii of CNT reinforced nanocomposite are predicted first using the representative volume element (RVE) method. CNTs are considered to have the periodic spatial distribution in the RVE and their 3D orientations are randomized using the *livelink* between COMSOL Multiphysics and the MATLAB. Thereafter, the effect of CNT reinforcement on the buckling behavior of simply-supported nanocomposite plate is predicted using the *plate* physics of COMSOL Multiphysics. The procedure to calculate the Young's modulus is verified by comparing the results of the single CNT reinforced RVE with the analytical solution obtained by the rule of mixtures. Buckling strength of the nanocomposite plate is also compared with the classical plate theory (CPT) based analytical result. It is concluded that the enhanced stiffness properties of the CNT-reinforced nanocomposite resulted in the increase of buckling strength of the nanocomposite plate.

Keywords: Carbon nanotube, Representative volume element, Elastic modulii, Buckling strength

1. Introduction

Carbon nanotubes (CNTs) discovered in 1991 by Iijima [1] are the frontier research area because of their extraordinary strength, resilience, stiffness and low density properties [2-4]. CNTs have attracted the attention of researchers from almost all fields, because of their superior electrical, thermal and mechanical properties, CNTs are potentially great reinforcing element in different matrix materials such as polymers, ceramics and metals, to enhance the overall properties of the resulting composite material. These CNTs are sp^2 bonded 3D structure of fullerene family, made of one atom thick rolled sheet which are stronger than the sp^3 bonded alkanes and diamonds that provide them unique properties. The buckling strength of these resulting nanocomposite plates are also studied by few authors using analytical solution based on first order shear deformation theory (FSDT) [5] and approximate solution based on element-free kp-Ritz method [6].

The aim of present paper is to predict the elastic properties of randomly oriented and periodically distributed CNT reinforced nanocomposite using 3-D nano scale representative volume element (RVE) based on continuum mechanics approach. Subsequently, the effect of CNT reinforcement on the buckling strength of the nanocomposite plate is also predicted. Perfect bonding is assumed between the nanofiller (i.e. CNT) and the matrix material. Strength of materials based rule of mixtures and analytical formula for buckling strength of the plate based on classical plate theory (CPT) are used to validate, respectively, the axial Young's modulus of the CNT reinforced nanocomposite material and the buckling strength of nanocomposite plate obtained from COMSOL Multiphysics.

2. Representative volume element

Multi-scale methods are required to deal with the wide length and time scales of nanocomposites that vary from nano to macro level, by integrating the molecular dynamics and continuum mechanics approaches. This has posed many challenges to all the researchers in the area. The concept of representative volume element, originally used for fiber reinforced composites [7], has also been carried forward in the characterization of nano scale materials. Liu and Chen [8] proposed three types of nanoscale RVE, namely cylindrical, square and hexagonal. It was shown that cylindrical RVE provide good prediction of elastic properties of CNT nanocomposite in the case of axisymmetric loading, but at the same time cylindrical RVEs tends to overestimate the volume fraction of nanofillers in a matrix material [9]. Square and hexagonal RVEs are used when nanofillers are distributed in a matrix material in square and hexagonal arrays, respectively. In the present study CNTs are considered to be oriented randomly and distributed periodically, therefore a square (cubical) RVE is considered to study the effect of CNT's reinforcement in a metal matrix on the buckling behavior of nanocomposite plate.

3. Analytical approach

Strength of materials based rule of mixtures (ROM), based on Reuss model, is a very good method for estimating the elastic modulus in axial direction, and because of its simplicity and accuracy, the ROM has been frequently used by many researchers [8-12] to validate their results. ROM doesn't predicts good results for transverse Young's modulii because it does not take into the account the geometry and dimensions of the reinforcement but considers only the volume fraction of reinforcement. Under the assumption of perfect bonding between the reinforcement and the matrix, following relationships describes the ROM, that are used to calculate the stiffness properties of the RVE.

$$E_1 = V_f E_f + (1 - V_f) E_m \tag{1}$$

$$E_2 = \frac{E_f E_m}{E_m V_f + (1 - V_f) E_f} \tag{2}$$

$$G_{12} = \frac{G_f G_m}{G_m V_f + G_f (1 - V_f)} \tag{3}$$

$$\nu_{12} = \nu_f V_f + \nu_m (1 - V_f) \tag{4}$$

Volume fraction of CNT in a matrix material is calculated as:

$$V_f = \frac{V_{CNT}}{V_{RVE}} = \frac{n\pi\left(r_0^2 - r_i^2\right)L_{CNT}}{\left(a^2 - \pi n r_i^2\right)L_{RVE}} \tag{5}$$

where r_i and r_o are the inner and outer radii of the CNTs; a denotes the side of square RVE; L_{CNT} and L_{RVE} represent the lengths of the CNT and RVE, respectively, and; n is the number of CNTs.

A single CNT reinforced RVE is modeled (i.e. n =1), to predict the finite element analysis (FEA) based results for elastic properties of the resulting nanocomposite, that are further validated with the corresponding results obtained by applying ROM, as specified in Eqs. (1-4). At the same time, the buckling strength of the plate made of nanocomposite material is calculated using COMSOL Multiphysics and that is validated with the corresponding results obtained from the analytical formula based on the classical plate theory (CPT).

For all edges simply supported, the critical buckling load of a plate is given as:

$$\lambda_{cr} = \frac{4\pi^2 D}{b^2} \tag{6}$$

where, $D = \dfrac{Eh^3}{12\left(1 - \nu^2\right)}$

where, b and h represent side and thickness of the square plate, respectively; E and ν are the Young's modulus and Poisson's ratio of the plate material, respectively.

4. Validation

For the study purpose Magnesium (Mg) is considered as the matrix material and that is reinforced with 1% of CNT to make a nancomposite material. Elastic properties of the reinforcement (i.e., CNT) and the matrix materials are given below:

For matrix: Young's modulus E_m = 45 GPa, Poisson's ratio, ν = 0.3.

For Carbon nanotube: Young's modulus E_f =1000 GPa, Poisson's ratio, ν = 0.3.

Dimensions of the CNT are taken as:

Outer radius, r_o =3.6 nm, Inner radius, r_i= 3.2 nm, Length, L_{CNT} =50 nm.

For a given volume fraction and $L_{CNT} = L_{RVE}$, the side of the RVE (made of a single CNT reinforced in the matrix material, as shown in Fig. 1) a can be calculated using Eq. (5). The finite element meshing of RVE using tetrahedron elements is performed using physics controlled feature of COMSOL MultiPhysics. The elastic properties of the nanocomposite are obtained by finite element analysis of the RVE subjected to different periodic displacement boundary conditions, as discussed in Ref. [7]. In the current study, perfect bonding is assumed between the reinforcement and the matrix to simplify the analysis. The effective elastic constants of the nanocomposite are extracted from the ratios of their respective volumetric averages of the stress and the strain.

The results of comparison between the present study (carried out on a single CNT-reinforced RVE) and the ROM are tabulated in Table 1. A good agreement between the values of E_1 and ν_{12} obtained from the FEA analysis and those obtained from ROM can be observed in Table 1. But as expected, there is deviation between the values of E_2, E_3 and G_{12} obtained in the present investigation from that calculated from the ROM.

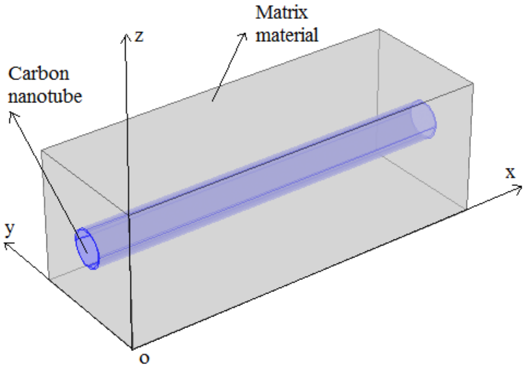


Figure 1 Single CNT RVE for the $v_f = 0.01$.

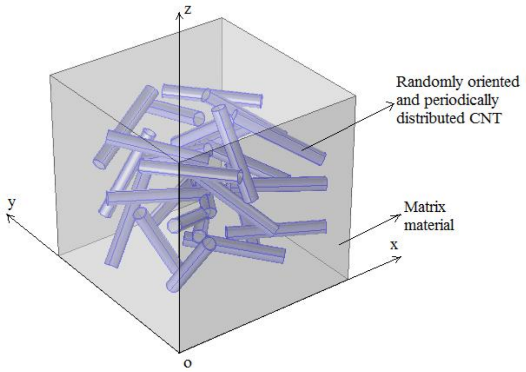


Figure 2. RVE consisting of randomly oriented and periodically distributed CNT for $v_f = 0.01$.

Table 1. Comparison of Elastic constants of CNT nanocomposite obtained in the present study and the ROM

Elastic Constants	FEA results	ROM
E_1	54.5510	54.5499
E_2=E_3	47.2526	45.4338
G_{12}= G_{13}	18.4449	17.4745
ν_{12}	0.2999	0.3000

5. Present Study

In the present study, a complete characterization of the nanocomposite (made of the same CNT-Mg materials combination) with periodically distributed and randomly oriented *n* CNTs is carried out. For this study, CNTs are given spatial periodic distribution and 3D random orientation in the matrix using *livelink* between the COMSOL Multiphysics and the MATLAB. To calculate the random orientation of each CNT, random numbers are generated using *randi* command of MATLAB. The modeled cubical RVE (having $L_{RVE} = a$ and L_{CNT} = 50nm) of the CNT-Mg nanocomposite (having 1 % volume fraction of CNT reinforcement) with periodic distribution and random orientation of *n* CNTs is shown in Fig. (2). Using the above validated procedure in Section 4, a complete characterization of this RVE for elastic properties is carried out. Subsequently, the buckling strength of the simply-supported plate made of the above characterized CNT-Mg nanocomposite material is studied using *plate* physics of COMSOL Multiphysics. The boundary conditions of a simply supported plate used in the study are shown in Fig. (3). Side of the square plate is taken as, b = 0.2 m and its thickness is taken as 0.004 m. Obtained results are compared with that obtained from Eq.(6).

6. Results and Discussion

The effective elastic properties of the CNT-Mg nanocomposite are listed in Table 2. There is approximately 7 % increment in the E_x, E_y and E_z normal elastic modulii relative to that of pure matrix material. Further, shear modulii G_{xz}, G_{yz} and G_{xy} are improved by 8 % as compared to the modulus of pure matrix material. Since, the obtained values of the nanocomposite mimic the isotropic behavior of actual randomly oriented CNT nanocomposite, thus an average values of extensional modulus, shear modulus and Poisson's ratio are considered in the present work to study the buckling behavior of nanocomposite plate. Evaluated average values of Elastic constants are given below:

E = 48.0508 GPa, G = 18.7858 GPa and ν = 0.3025

Buckling strength of pure Mg plate and CNT-Mg nanocomposite plate obtained from CPT based analytical solution using Eq. (6) and FEM solution using COMSOL are listed in Table 3. First four mode shapes of the CNT-Mg nanocomposite plate are shown in Fig. (4). The deviation found by the two method can be attributed to the fact that CPT doesn't consider the effect of shear deformation through the thickness of the plate whereas *plate* physics section of COMSOL MultiPhysics considers the same and works on Mindlin-Reissner theory of plates which is an extension of CPT. As compared to pure Mg plate, approximately 7 % increment in the buckling strength of the nanocomposite plate is obtained which can be further improved by increasing the percentage of CNT. Therefore, the enhanced stiffness properties of nanocomposite have resulted in the enhanced buckling strength of nanocomposite plate.

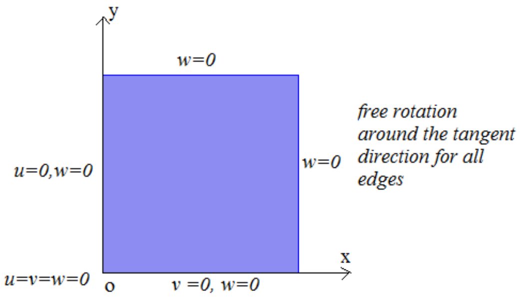


Figure 3. Boundary conditions for the all edges simply supported plate

7. Conclusion

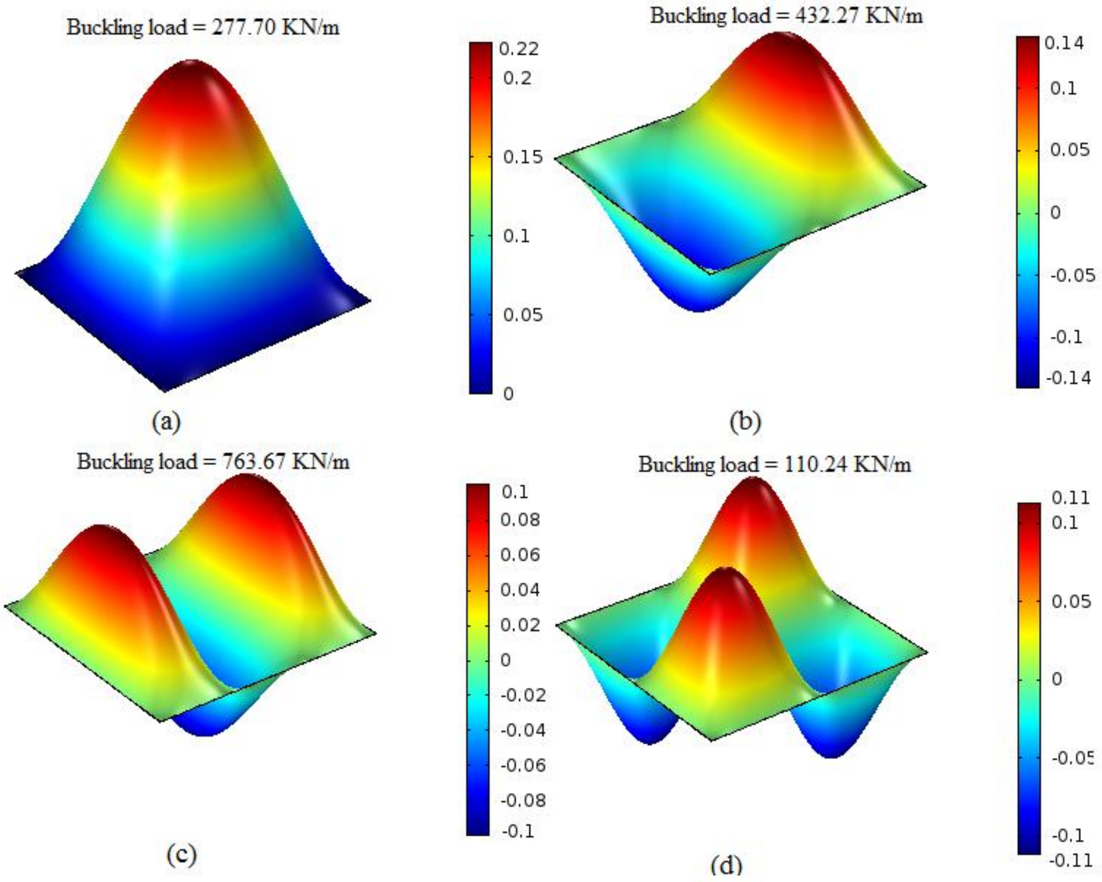
Effective elastic constants of randomly oriented and periodically distributed CNT reinforced Mg nanocomposite are predicted using cubical representative volume element subjected to different periodic boundary conditions. The obtained model shows the isotropic behavior that can mimic the actually developed isotropic nanocomposites. Finite element method is used to perform the analysis using COMSOL Multiphysics software. The procedure is validated by comparing FEA result for the axial modulus with the corresponding analytical result obtained from mechanics of solid based rule of mixtures (ROM). Complete characterization in terms of various elastic moduli of CNT nanocomposite is done. The effect of CNT reinforcement on the buckling behavior of a simply supported square plate is also predicted using the *plate* physics section of COMSOL Multophysics. Based on the present study, it can be concluded that reinforcement of CNTs enhances the stiffness properties of the metal matrix which in turn increases the buckling strength of the plate.

Table 2 Effective elastic properties of randomly oriented CNT-Mg nanocomposite

E_x	E_y	E_z	G_{xy}	G_{xz}	G_{yz}	ν_{xy}	ν_{xz}	ν_{yz}
48.2329	48.1131	47.8064	18.9878	18.6932	18.6764	0.2994	0.3036	0.3045

Table 3 Comparison of buckling strengths of pure Mg and CNT-Mg nanocomposite (having 1 % reinforcements) obtained using the COMSOL Multiphysics and the analytical formula based on CPT.

Plate Material	COMSOL Multiphysics (KN/m)	Analytical results based on CPT (KN/m)
Mg	259.64	260.2973
CNT-Mg Nanocomposite	277.70	278.4051


Buckling load = 277.70 KN/m

Buckling load = 432.27 KN/m

Buckling load = 763.67 KN/m

Buckling load = 110.24 KN/m

(a) (b) (c) (d)

Figure 4. (a-d) First four mode shapes of CNT-Mg nanocomposites plate having 1% CNT reinforcement with *a/h* =50.

8. References

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