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Finite Element Modeling of the Vibrational Behavior of Single-Walled Silicon Carbide Nanotube/Polymer Nanocomposites

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ABSTRACT
The multi-scale finite element method is used to study the vibrational characteristics of polymer matrix reinforced by single-walled silicon carbide nanotubes. For this purpose, the nanoscale finite element method is employed to simulate the nanotubes at the nanoscale. While, the polymer is considered as a continuum at the larger scale. The polymer nanotube interphase is simulated by spring elements. The natural frequencies of nanocomposites with different nanotube volume percentages are computed. Besides, the influences of nanotube geometrical parameters on the vibrational characteristics of the nanocomposites are evaluated. It is shown that reinforcing polymer matrix by single-walled silicon carbide nanotubes leads to increasing the natural frequency compared to neat resin. Increasing the length of the nanotubes at the same diameter results in increasing the difference between the frequencies of nanocomposite and pure polymer. Besides, it is observed that clamped-free nanocomposites experience a larger increase in the presence of the nanotubes than clamped-clamped nanotube reinforced polymers.

Keywords : Finite element method; Vibrational behavior; Single-walled silicon carbide nanotube; Polymer matrix; Nanocomposites.

1 INTRODUCTION

AFTER publishing of the first paper on the carbon nanotubes (CNTs) by Iijima [1], they found vast potential applications in different fields such as nano-transistors, nano-fillers, semiconductors, hydrogen storage devices, structural materials, molecular sensors, field-emission-based displays, and fuel cells, to name just a few [2]. This is because of their extraordinary electronic and mechanical properties, such as the high elastic modulus, tensile strength, aspect ratio, large surface area, low density and resistance to failure [3]. It has been observed that the mechanical, electrical and thermal properties of polymeric composites experience significant improvement by adding a small amount of CNTs in the polymer matrices [4-6]. Although experimental methods have also been used by some researchers to study the mechanical behavior of nanocomposites [7-11], due to the difficulty of the experiments at the scale of nano, the mechanical behavior of CNT/polymer nanocomposites have been studied by

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different theoretical approaches such as finite element (FE) method and molecular dynamics (MD) simulations. MD simulations were used by Frankland et al. [12] to evaluate the mechanical properties of single-walled carbon nanotube (SWCNT)/polyethylene nanocomposites. It was shown that the unlike short SWCNTs, mechanical properties of nanocomposites significantly ascend by including long nanotubes. The effect of SWCNT inclusion on the mechanical behavior of poly (methyl methacrylate) (PMMA) and poly{(m -phenylene-vinylene)-co -[(2,5-dioctoxy- p-phenylene) vinylene]} (PmPV) [6] and Epon 862 [13] matrices was also studied by MD simulations. Mokashi et al. [14] represented that the mechanical properties of crystalline and amorphous polypropylene experience moderate and significant increase, respectively, by embedding SWCNTs. Using MD simulations, Tsai et al. [15] evaluated the non-bonded energy between the SWCNT and polyimide matrix. The MD simulations and continuum micromechanics were employed by Yang et al. [16] to propose a multiscale method which can be used to investigate the elastic behavior of SWCNT/polypropylene nanocomposites. A MD based hierarchical multiscale model was also proposed by them to investigate the elastoplastic behavior of SWCNTs/polypropylene nanocomposites [17]. MD simulations were used by Bohlén and Bolton [18] to study the effect of embedding pure SWCNTs functionalized SWCNTs on the mechanical properties of Poly(vinylidene fluoride) (PVDF) matrix. They showed that embedding pure SWCNTs does not affect the mechanical properties of PVDF significantly. However, the mechanical properties of polymer affect by embedding functionalized SWCNTs considerably.

By using MD simulations, the mechanical properties of SWCNT/poly (phenylacetylene) nanocomposites were investigated by Rouhi et al. [19]. It was observed that the transverse elastic modulus of the poly (phenylacetylene) nanocomposites does not significantly change in the presence of the SWCNTs. They also observed a peak near the nanotube surface in curve of the density of polymer surrounding the nanotube surface [20]. They proposed a FE method based on the MD simulations of SWCNT/polyethylene and polyketone nanocomposites which were used to investigate the longitudinal tensile behavior of nanocomposites [21]. In addition to MD simulations, the mechanical properties of SWCNT/polymer nanocomposites have been investigated by FE method. Simulating the C-C bonds and an der Waals (vDW) interactions between SWCNT and polymer matrix by beam and truss elements, Li and Chou [22] studied the compressive behavior of the nanocomposites by Georgantzinos et al. [23-24] simulated vdW interactions by spring elements. Besides, Shokrieh and Rafiee [25-26] used a full 3D FE model to investigate the longitudinal, transverse and shear moduli of SWCNT reinforced polymers. Considering the SWCNT, polymer matrix and SWCNT/polymer interface, Wernik and Meguid [27-28] proposed a nonlinear representative volume element (RVE) in which the constant of spring representing the vdW interactions between polymer and SWCNTs changes during the simulations by changing the distance between the atoms. The polymer matrix has been simulated as a continuum media in all of the mentioned works. Considering the discrete structure of polymer matrix, Meguid et al. [29] proposed a full atomistic FE method.

Like CNT, silicon carbide nanotubes (SiCNTs) possess great mechanical properties which can lead their application in the nanotube reinforced polymer. Young's modulus of SiCNTs has been predicted as $465GPa$ and $540GPa$ for the wall thicknesses of $0.30nm$ and $0.90nm$, respectively [30]. It has been represented that the elastic properties of single-walled SiCNTs (SWSiCNTs) depend on nanotube diameter [31]. Besides, they have large buckling forces and great vibrational behavior [32-33]. SWSiCNTs are used here to raise the vibrational behavior of the polymer matrix. The effects of nanotube geometrical parameters, chirality and volume fraction on the frequencies of SWSiCNT/polymer nanocomposites are investigated. Besides, the vibrational characteristics of clamped-clamped and clamped-free nanocomposites are explored. The effect of RVE cross sectional shape on the fundamental natural frequencies of nanocomposites is also studied.

2 MODELING APPROACH

Fig. 1 shows the employed model to simulate the SWSiCNTs. In the utilized approach, the Si-C bonds are modeled by using beam elements whose properties are obtained by the analogy of energy terms in molecular and structural mechanics. Utilizing this method, Young's modulus, shear modulus, diameter and length of these beam elements are obtained as $E = 2.9372\times10^{-8} N / \mathring{A}^2, G = 2.6256\times10^{-8} N / \mathring{A}^2, d = 1.7971\mathring{A}$ and $L = 1.786\mathring{A}$, respectively [32-34]. On the other hand, the mass elements with the values of $4.6646\times10^{-26} kg$ and $1.9943\times10^{-26} kg$ are used at the corners of beam elements to simulate the Si and C atoms, respectively considering the isotropic and homogenous behavior of the matrix and its large volume compared to the nanotubes, it is simulated as a continuum media.

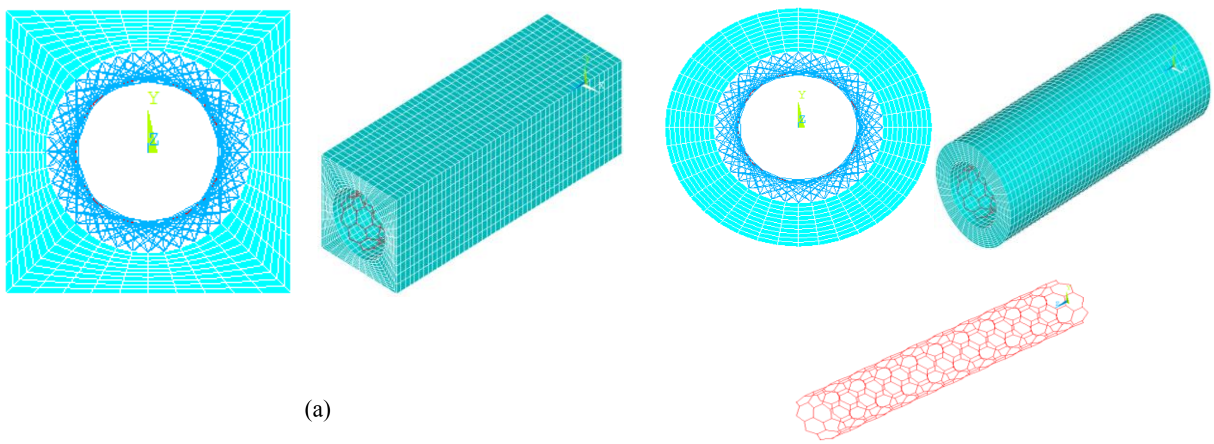
Finally, nonbonding atomic interactions in the interphase region are governed by the van der Waals (vdW) interaction which is expressed by using the 6–12 Lennard–Jones potential function as:

$$U(R) = 4\varepsilon\left[\left(\frac{\sigma}{R}\right)^{12} - \left(\frac{\sigma}{R}\right)^{6}\right] \tag{1}$$

where R is the distance between atoms and ε and σ are Lennard-Jones parameters which depend on two interacting atoms. Spring elements are used here to model the nonbonding interactions in the interphase region. To obtain the stiffness of the spring, one should differentiate Eq. (1) with respect to R. Therefore:

$$k_{vdw} \frac{dU}{dR} = 24\varepsilon\left(26\frac{\sigma^{12}}{R^{14}} - 7\frac{\sigma^{6}}{R^{8}}\right) \tag{2}$$

Substituting the values of ε and σ in the above equation, the spring stiffness is computed as a function of interatomic distance. Fig. 1 shows the schematic of the simulated RVEs along with different utilized elements.

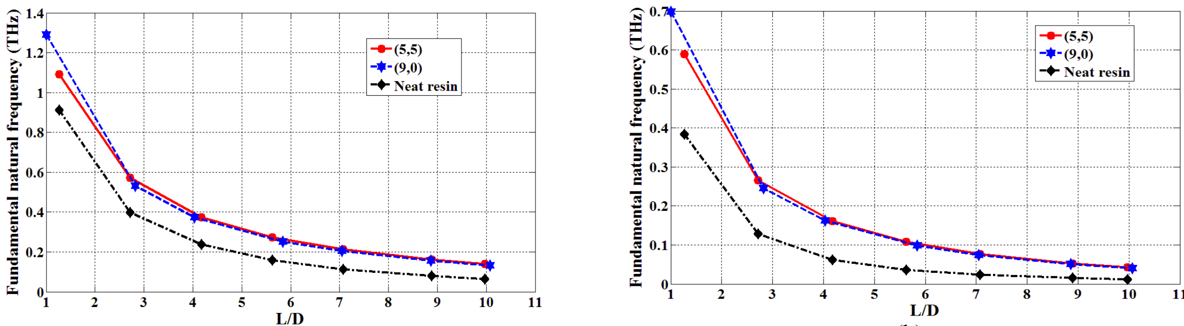


(a) (b)

Fig.1
Schematics of (a) cubic and (b) cylindrical RVEs.

3 RESULTS AND DISCUSSION

The frequencies of polymer matrix reinforced by SWSiCNTs are obtained by using the prescribed approach. An epoxy resin with Young's modulus, Poisson's ratio and density of $10GPa$, 0.3 and $890kg/m^3$ is considered as the matrix. Fig. 2 shows the fundamental natural frequencies of the polymer matrices reinforced by SWSiCNTs. The nanotube volume percentage is selected as 40%. It can be seen that adding SWSiCNTs to the polymer matrix leads to increasing the frequencies compared to the neat resin. For example, reinforcing the clamped-clamped polymer matrix by (5,5) and (9,0) SWSiCNTs with the aspect ratio of 4 leads to 57.61% and 56.95% increase in the fundamental natural frequencies. For the clamped-free boundary conditions, the corresponding values are 159.85% and 160.37%, respectively. Therefore, it can be concluded that the effect of reinforcing polymer matrix by SWSiCNTs is more significant under the clamped-free boundary conditions. Besides, with the aspect ratio of 7, the corresponding values of clamped-clamped RVEs increase to 88.16% and 81.14%, respectively. The percentages of increase in the fundamental natural frequencies of clamped-free nanocomposites are 229.83% and 216.33%, respectively. So, one can conclude that increasing the aspect ratio of the employed SWSiCNT to reinforce the polymer matrix leads to increasing the fundamental natural frequencies of the SWSiCNT/polymer nanocomposites.

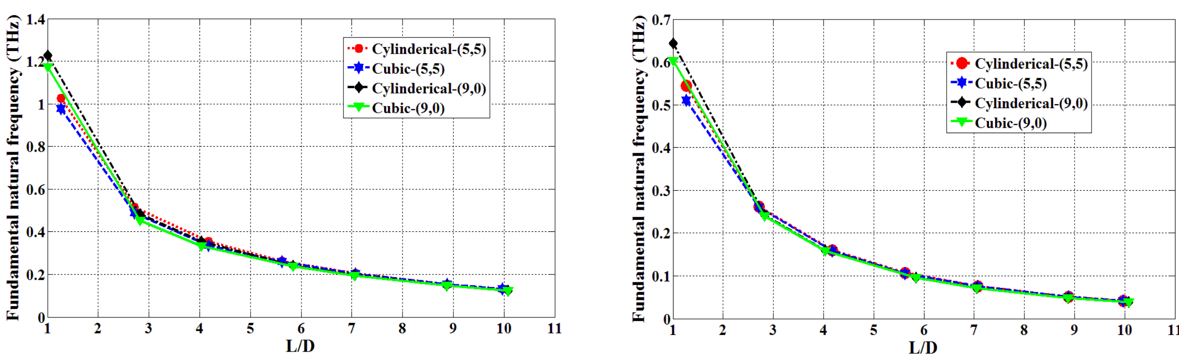


(a) (b)

Fig.2
Comparison of the frequencies of neat resin and SWSiCNT reinforced polymer matrix; Cylindrical RVEs under (a) clamped-clamped and (b) clamped-free boundary conditions, nanotube volume percent = 40%.

3.1 Effect of cross sectional shape of RVE

In this section, the effect of RVE shape on the computed natural frequencies is studied. Two different RVEs are used with the square and circular cross sections. The former and latter RVEs are mentioned as cubic and cylindrical RVEs, respectively. Fig. 3 shows the fundamental natural frequencies of the cubic and cylindrical RVEs reinforced by (5,5) and (9,0) SWSiCNTs. The nanotube volume percentage is chosen as 30%. It can be seen that, except a small region at the initial sections of the graphs, the effect of RVE cross sectional shape on the computed frequencies of the nanocomposites can be neglected.



(a) (b)

Fig.3
Comparison the frequencies of cylindrical and cubic RVEs reinforced by SWSiCNT; RVEs under (a) clamped-clamped and (b) clamped-free boundary conditions, nanotube volume percent = 30%.

3.2 Effect of SWSiCNT chirality and diameter

To study the effect of nanotube diameter and chirality on the fundamental natural frequencies of the SWSiCNTs, four different nanotubes are selected here whose chiralities and diameters are given in Table 1. Fig. 4 shows the fundamental natural frequencies of the polymer matrix reinforced by the selected nanotubes. Due to insignificancy of the RVE shape, the cylindrical RVE is used here. Besides, the SWSiCNT volume percentage is 40%. Comparing the curves associated with the frequencies of polymer matrix reinforced by armchair and zigzag SWSiCNTs with a same diameter, it can be seen that the effect of chirality on the vibrational behavior of SWSiCNT/polymer nanocomposite is not important. It can be seen that the curves associated with (10,10) and (17,0) nanotube are approximately coincident. Therefore, it can be concluded that the effect of chirality is even smaller for larger diameters.

Besides, it is observed that the polymer matrix reinforced by SWSiCNTs of smaller diameters have larger frequencies. For example the frequency of a clamped-clamped RVE reinforced by (5,5) SWSiCNT with the aspect ratio of 4 is equal to 0.374 *TPa* which is 99% larger than the frequency of the corresponding RVE reinforced by

(10,10) SWSiCNT (f=0.188 *TPa*). These values are 0.162 *TPa* and 0.077 *TPa*, respectively. It means that the frequency of (5,5) SWSiCNT/polymer nanocomposite is 110% larger than that of (10,10) SWSiCNT/polymer nanocomposite. So, one can conclude that increasing the nanotube aspect ratio leads to strengthening the effect of nanotube diameter on the nanocomposite vibrational behavior.

Table 1
Geometrical parameters of the utilized SWSiCNTs for polymer reinforcement.

Armchair		Zigzag	
Chirality	Diameter ($\mathring{A}$)	Chirality	Diameter ($\mathring{A}$)
(5,5)	8.53	(9,0)	8.86
(10,10)	17.06	(17,0)	16.74

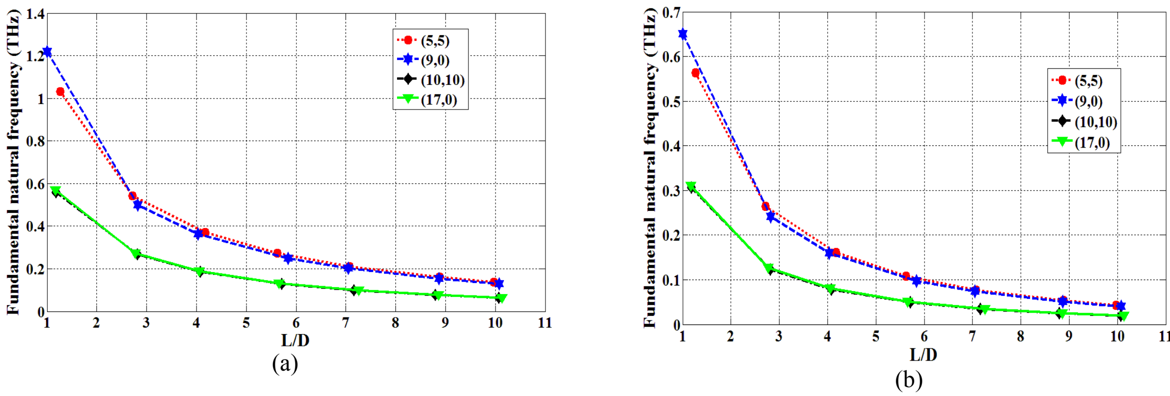


Fig.4
Comparison the frequencies RVEs reinforced by SWSiCNT with different chiralities and diameters; Cubic RVEs under (a) clamped-clamped and (b) clamped-free boundary conditions, nanotube volume percent = 40%.

3.3 Effect of SWSiCNT volume fraction

Now, the effect of SWSiCNT volume fraction on the fundamental natural frequency of the SWSiCNT reinforced polymer is investigated. To this end, three different volume percentages, including 30%, 40 and 50% are selected. Fig. 5 shows the fundamental natural frequencies of polymer matrix reinforced by different SWSiCNT volume percentages. It can be seen that the nanocomposites with larger nanotube volume fractions possess larger frequencies. The effect of volume fraction is more significant for clamped-clamped nanocomposites. Besides, increasing the nanotube aspect ratio leads to reducing the influence of SWSiCNT volume fraction on the fundamental natural frequencies of SWSiCNT/polymer nanocomposite.

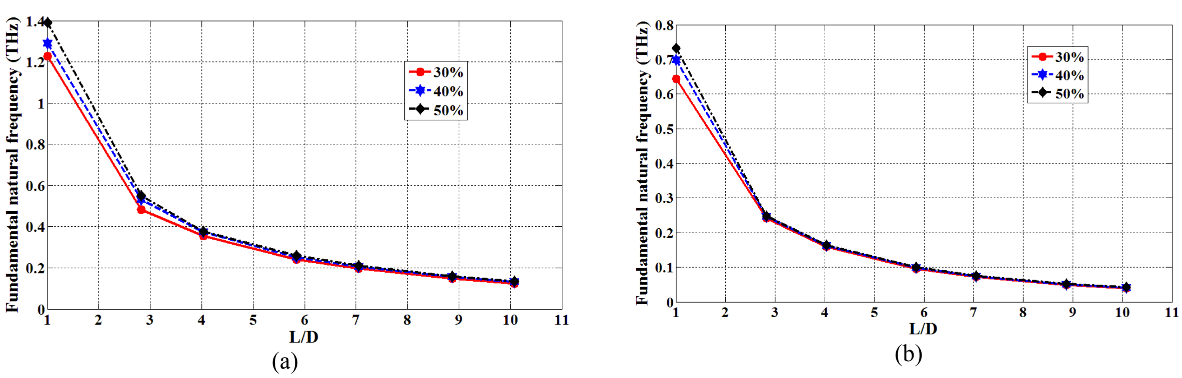


Fig.5
Comparison the frequencies RVEs reinforced by a (9,0) SWSiCNT with different volume fractions; Cylindrical RVEs under (a) clamped-clamped and (b) clamped-free boundary conditions.

3.4 Effect of boundary conditions

The effect of boundary conditions on the 1*st* and 5*th* natural frequencies of SWSiCNT reinforced polymer can be evaluated from Fig. 6. Here, a (5,5) SWSiCNT with the volume fraction of 30% is used to reinforce the cubic polymer matrix. It can be seen that for both of the boundary conditions, the difference between the frequencies decreases by increasing the aspect ratio. Besides, the first and fifth frequencies of clamped-clamped nanocomposites are larger than those of clamped-free nanocomposites. The difference is not significantly affected by increasing the nanotube aspect ratio.

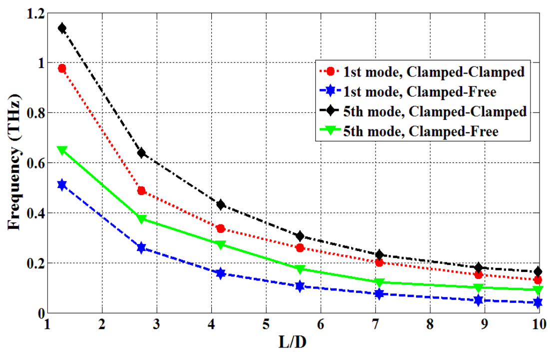


Fig.6
Comparison the first and fifth frequencies cubic RVEs reinforced by a (5,5) SWSiCNT under different boundary conditions; nanotube volume percent = 30%.

3.5 Higher modes

The first ten frequencies of (5,5) and (10,10) SWSiCNTs reinforced polymers are compared in Fig. 7 for different nanotube volume fractions. The cross sectional shape of the RVEs are considered as circle. Besides, the nanotube aspect ratio is selected as 4. It is seen that under both of the clamped-clamped and clamped-free boundary conditions, all of the frequencies of nanocomposites reinforced by nanotubes with larger diameters are larger than those of nanocomposites reinforced by nanotubes reinforced by nanotubes with smaller diameters. Besides, after the initial parts of the curves in which the frequencies of RVEs with smaller nanotube volume percents are smaller than those of RVEs with larger volume fractions, the order of curves would be changed. Fig. 8 shows the effect of nanotube chirality on the first ten frequencies of SWSiCNTs/polymer nanocomposites. It can be seen that as the fundamental natural frequency, the effect nanotube chirality on the higher frequencies of the SWSiCNT reinforced polymers is not considerable.

The first ten mode shapes of cubic and cylindrical RVEs reinforced by a (9,0) SWSiCNT are shown in Figs. 9-12. The RVEs are under clamped-clamped and clamped-free boundary conditions. Interestingly, the cubic RVEs experience the same mode shapes as the correspondig cylindrical RVEs which confirms the independence of the vibrational behavior of SWSiCNT/polymer nanocomposites to the RVE shape.

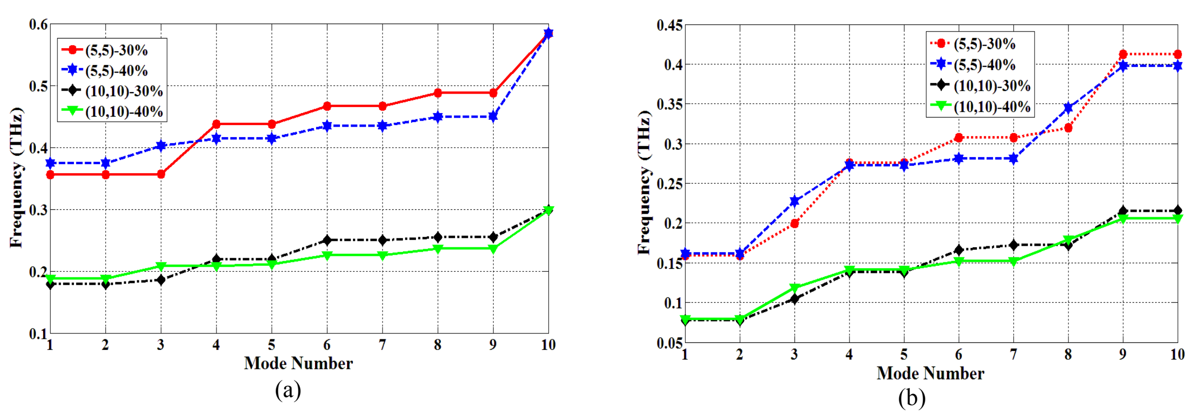
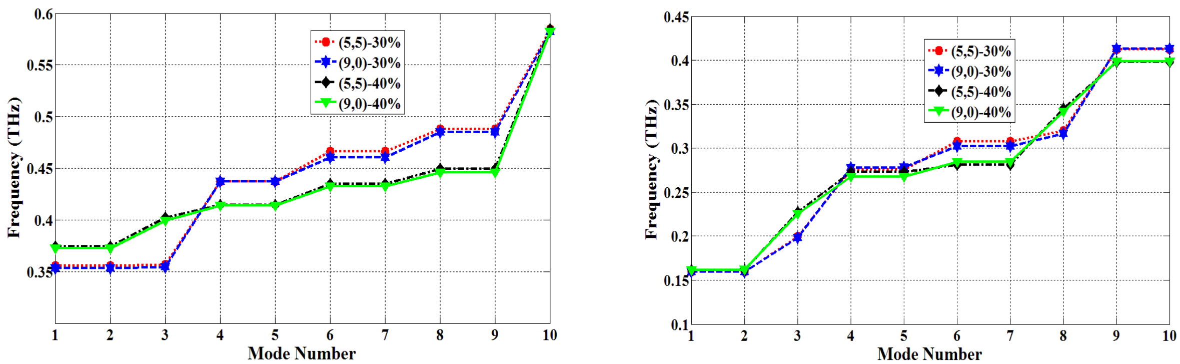
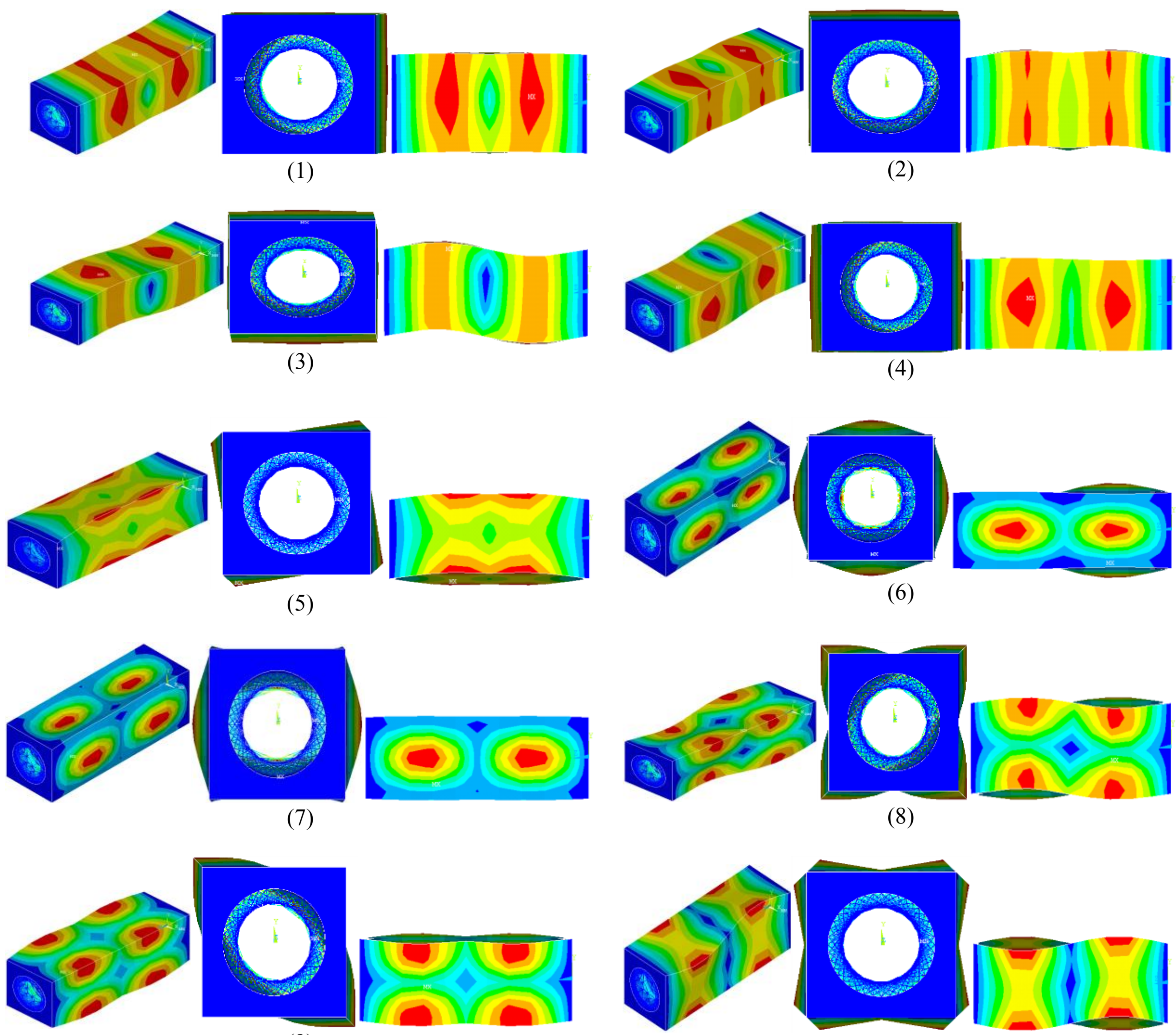


Fig.7
Comparison the first ten frequencies of RVEs reinforced by (5,5) and (10,10) SWSiCNT with the volume percents of 30% and 40%; Cylindrical RVEs under (a) clamped-clamped and (b) clamped-free boundary conditions, $L/D=4$.



(a) (b)

Fig.8
Comparison the first ten frequencies of RVEs reinforced by (5,5) and (9,0) SWSiCNT with the volume percents of 30% and 40%; Cylindrical RVEs under (a) clamped-clamped and (b) clamped-free boundary conditions, $L/D=4$.



(1) (2) (3) (4) (5) (6) (7) (8) (9) (10)

Fig.9
First ten mode shapes of cubic RVE reinforced by (9,0) SWSiCNT under clamped-clamped boundary conditions.

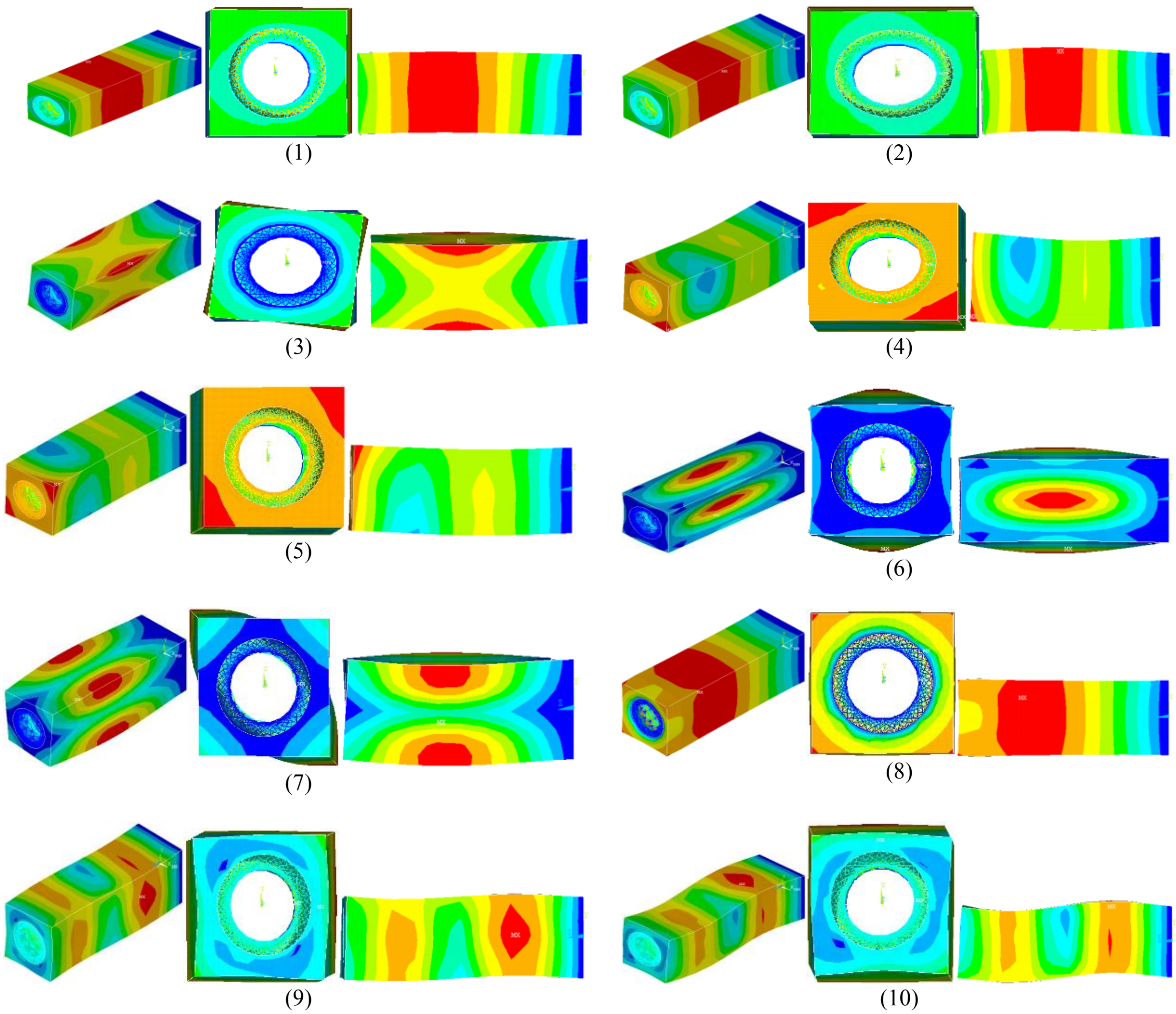
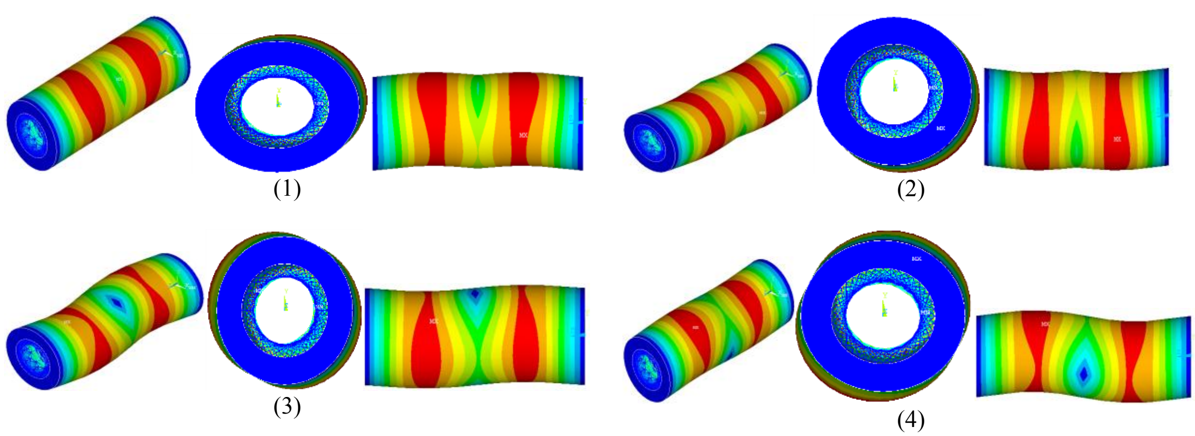


Fig.10
First ten mode shapes of cubic RVE reinforced by (9,0) SWSiCNT under clamped-free boundary conditions.



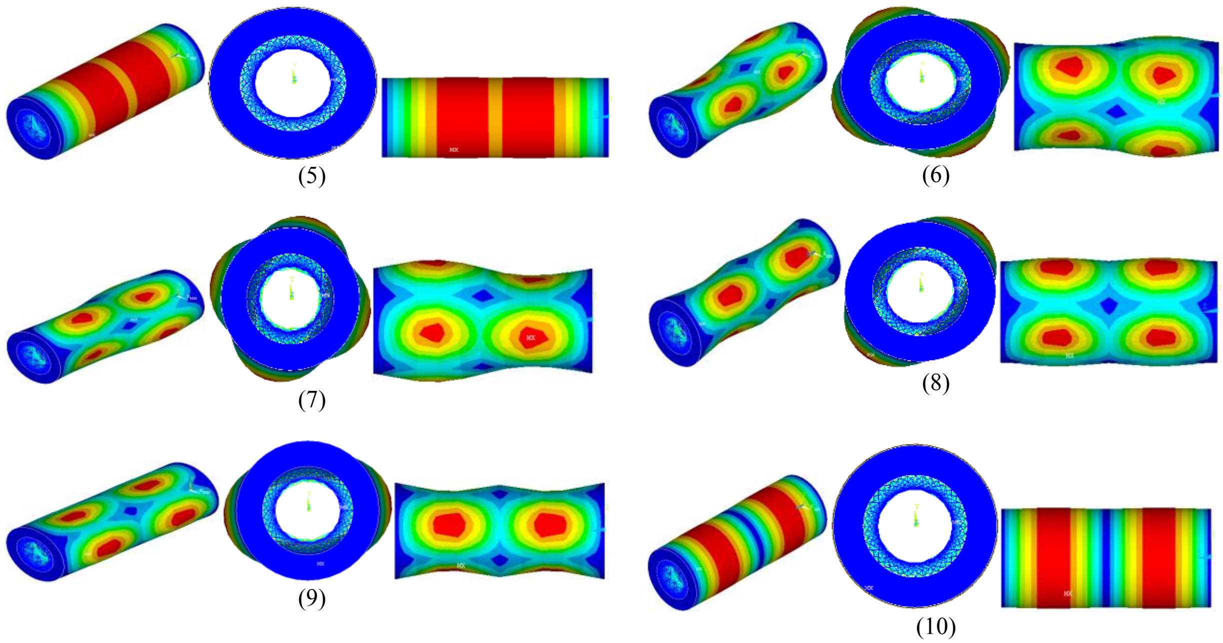
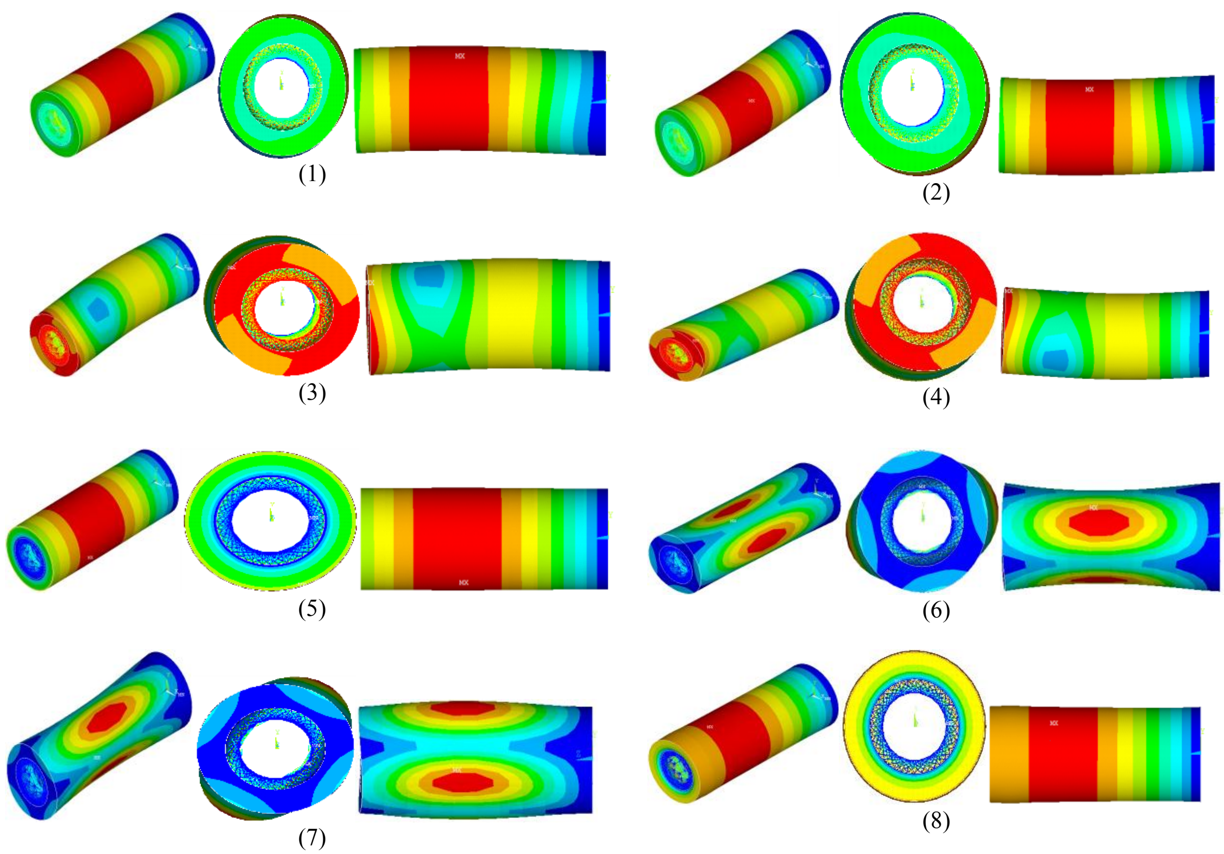
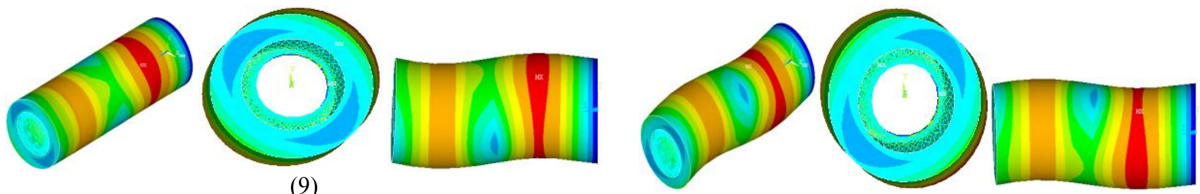


Fig.11
First ten mode shapes of cylindrical RVE reinforced by (9,0) SWSiCNT under clamped-clamped boundary conditions.





(9) (10)

Fig.12
First ten mode shapes of cylindrical RVE reinforced by (9,0) SWSiCNT under clamped-free boundary conditions.

4 CONCLUSIONS

In this paper, using FE method the frequencies of SWSiCNT/polymer nanocompositeswere computed. Comparing the frequencies of cubic and cylindrical RVEs, it was shown that the vibrational behavior of SWSiCNT reinforced nanocomposite is not significantly affected by the cross sectional shape of the RVE. It was shown that SWSiCNT with smaller diameters are more efficient to ascend the vibrational characteristics of the nanocomposites. Besides, the frequencies of the SWSiCNT/polymer nanocomposites are not significantly affected by the chirality of the nanotubes. Comparing the frequencies of nanocomposites reinforced by different nanotube volume fractions, it was revealed that the effect of SWSiCNT volume percentage on the natural frequencies of SWSiCNT/polymer nanocomposites is more significant for clamped-clamped RVEs than clamped-free ones. However, for both of the boundary conditions this dependence diminishes for long nanotubes.

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