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1. Introduction

As it is known, high damping is an important factor for all machine elements; therefore, it is necessary to develop structural components with a high level of mechanical damping. High loss factor polymers have been the most frequently used in modern damping applications [1–5]. These existing damping materials have offered improved damping performance for structural components and systems. But there is a need to develop advanced materials for damping applications, that can overcome these limitations. Recent researches effort in this direction have been much focused on the development of polymer damping materials based on nanocomposites in which nanotubes, nanofibers or nanoparticles are embedded in polymer substrates and much promising results have been established [6].

Continuum mechanics principles have been assumed to be valid and applied to study the mechanical properties of nanotubes [7]. While most of the researches on nanocomposites with carbon nanotubes focus on elastic properties, relatively little effort to date has been put in the studies of their damping characteristics. In fact, there exists a great potential in developing nanocomposites with high damping capacity using carbon nanotubes since the interfacial slip between nanotubes and polymer resin is considered. The nanocomposites damping ratio is calculated by evaluating the dissipation energy of nanocomposite. Also, the influence of different parameters such as volume fraction and length on the natural frequencies and damping characteristics of nanocomposite is investigated. Results show that of increasing volume fractions the natural frequency increases. Finally a relation between damping ratio and natural frequencies is obtained and it is found that second natural frequency increase due to increasing damping ratios.

In this paper first a vibration model of nanocomposites is obtained, then that nanocomposites structural damping characteristics are investigated, with focus on analyzing the interfacial interaction between the carbon nanotubes (CNTs) and the polymer resin. The concept of interfacial “stick–slip” frictional motion between the nanotubes and the resin is considered. The nanocomposites damping ratio is calculated by evaluating the dissipation energy of nanocomposite. Also, the influence of different parameters such as volume fraction and length on the natural frequencies and damping characteristics of nanocomposite is investigated. Results show that of increasing volume fractions the natural frequency increases. Finally a relation between damping ratio and natural frequencies is obtained and it is found that second natural frequency increase due to increasing damping ratios.

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atomistic scale and analyzed the matrix deformation using the continuum FE method. The van der Waals interactions between carbon atoms and the finite element nodes of the matrix were simulated using truss rods. Odegard and coworkers [10,11] developed an equivalent-continuum modeling method for simulating large amorphous organic-based materials such as polymers, carbon nanotubes and polymer nanocomposites. This method consists of three steps; namely, the establishment of an representative volume element (RVE) of the molecular and effective-continuum model, the establishment of a constitutive relationship for the effective-continuum model and the equation of the potential energies of deformation for identical boundary conditions. From the above short overview, it is obvious that there is still a need for developing flexible multi-scale approaches that will efficiently consider the nanotube behavior at the nanoscale being at the same time able to model carbon nanotube-reinforced composites at the meso- or the microscale.

In this paper a multi-scale model for polymer composites containing single walled carbon nanotubes (SWCNTs) is presented, and based on the interfacial stick–slip between CNTs and polymer resin, structural damping characteristics were predicted. The influence of the nanocomposites parameters on its mode shapes and natural frequencies was obtained.

2. Modeling

A representative volume element (RVE) of nanocomposite was modeled as Fig. 1. Zig-zag SWCNT was modeled considering the force interactions between its atoms, with the method that Li and Chou [12] have developed between the carbon nanotube molecular network and structural continuum mechanics. The Young modulus of the modeled nanotube is 1–1.5 TPa and this quantity was validated by previous researches [12–15]. Carbon atoms in the nanotube were meshed with structural mass (MASS21 in ANSYS) which is a point element having up to six degrees of freedom: translations in the nodal x, y, and z directions and rotations about the nodal x, y, and z axes and its mass is equal to carbon atoms mass number. A nanotube and its elements is shown in Fig. 2.

A cylinder polymer with specific material properties (Young modulus = 3.3 GPa and Poisson’s ratio = 0.3) was also modeled. An ANSYS APDL code was written to model the interaction between nanotube and matrix. A 3D non-linear spring element (COMBIN39) was considered between the matrix’s inner nodes (which were meshed by SOLID45) and the nanotubes nodes. COMBIN39 elements exerted the van der Waals forces between polymer’s atoms and carbon’s atoms of nanotube [16]. As Fig. 3 shows, thousands of elements modeled the interface. Actually, the bonding between embedded CNT and its surrounding polymer takes place through VDW interactions. The van der Waals forces obtained from the Lennard–Jones potential [17]. The van der Waal’s force is a non-linear force and it is zero when the interatomic distance is equal or greater than 0.85 nm as is shown in Fig. 4.

Eq. (1) describes the relation between the van der Waal’s force and interatomic distance [18]:

\[ F_{\text{vdw}} = -\frac{\varepsilon}{r} \left( -12 \left( \frac{\sigma}{r} \right)^6 + 6 \left( \frac{\sigma}{r} \right)^{12} \right) \]

where \( \varepsilon \) and \( \sigma \) are the Lennard–Jones parameters with value of 0.4492 kJ/mol and 0.3825 nm, respectively [19–22] and \( r \) are interatomic distances. The VDW interactions between carbon atoms of CNT and the nodes of inner surface of the surrounding resin, is modeled using a 3D non-linear spring. COMBIN39 element is used for this purpose and the parameters are adjusted to obtain translational spring [23]. An element between those nodes distance is lower than 0.85 nm. For simplification, the spring elements are only created between carbon atoms of the CNT and the inner surface of the resin. The thickness of CNT’s wall is selected as 0.34 nm and center of the carbon atoms in the CNT are placed at the midsection of the tube thickness. The innermost layer of the resin is assumed to be located at the same position of the outer surface.

3. Damping

3.1. Concept of “stick–slip” behavior

The stick–slip mechanism in a nanocomposite is shown in Fig. 5. When a normal tensile stress is applied to a composite, it starts elongating. As a result of the applied stress, the resin starts applying a shear stress, \( \tau \) on the nanotube, thus causing the load to be transferred to nanotubes. Consequently, normal strain starts appearing in nanotubes and they start elongating accordingly. When the applied stress is small, the nanotube remains bonded to the matrix (sticking phase). Both the resin and the nanotube move together during this phase and the strains are equal in both epoxy resin and nanotube. As the applied stress is increased, the shear stress on CNT increases. At a certain value of shear stress (called the critical shear stress, \( \tau_{cr} \)), the nanotube debonds from the resin. When the shear stress on the nanotube increases beyond this value (as a result of increased applied stress), the epoxy starts flowing over the surface of the nanotube. The strain in the nanotube remains constant at its maximum level while the strain in the epoxy increases (slipping phase). In this phase, there is no transfer load between CNT and matrix, and because of this energy dissipation due to slippage occurs which resulted to structural damping.

3.2. Investigating loss factor and damping ratio

As described above, one of the important causes of damping in nanotube-reinforced composites is the friction between nanotube and matrix.

Dissipated energy via interfacial movement of nanotube and matrix is equivalent to the shear force and the differential displacement between tube and matrix. For investigating loss factor, \( \eta \), total dissipation energy \( (U) \), and dissipation energy \( (\Delta U) \), equations [2] can be used [24].

\[ \eta = \sin^{-1} \left( \frac{\Delta U}{2\pi U_{\text{diss}}} \right) \]

\[ U_{\text{diss}} = \int_{\gamma} \left( \frac{\sigma d \gamma}{2} \right) dv \]

\[ \Delta U = 2\sigma_{\text{max}} \cdot (2\pi r^2) \cdot (\varepsilon_0 - \varepsilon_2) \]
where $r$ is the radius of the nanotube; $l_2$ is the length of the nanotube; $e_0$ is the strain of matrix material due to loading; $e_z$ is the bonding stress associated with longitudinal shear between nanotube and matrix material; $\tau_{\text{max}}$ is the critical shear stress which was described before and is obtained as follows [24]:

$$
\tau_{\text{max}}(z) = E^{eq} e_z \cdot \int_0^{l_2} \frac{\sinh(\beta(\frac{z}{2} - z))}{\cosh(\frac{z}{2})} \, dz \cdot \sqrt{\frac{G_0}{E^{eq} l_2}} \cdot \frac{1}{2 \ln(\frac{1}{2})}
$$

Fig. 4. Variation of VDW force versus interatomic distances [18].

$$
\tau_{\text{max}} = \frac{\tau_{\text{max}} \cdot l_2 / 2}{E^{eq} \cdot \int_0^{l_2} \frac{\sinh(\beta(\frac{z}{2} - z))}{\cosh(\frac{z}{2})} \, dz} \cdot \sqrt{\frac{G_0}{E^{eq} l_2 \ln(\frac{1}{2})}}
$$

So $e_z$ is the strain between nanotube and matrix material that can be calculated as follows:

$$
e_z = \frac{\tau_{\text{max}} \cdot l_2 / 2}{E^{eq} \cdot \int_0^{l_2} \frac{\sinh(\beta(\frac{z}{2} - z))}{\cosh(\frac{z}{2})} \, dz} \cdot \sqrt{\frac{G_0}{E^{eq} \ln(\frac{1}{2})}}
$$

where $R$ is the radius of composite; $G$ is the shear modulus of matrix material ($G_0 = 0.2$ GPa for polymers) and $E^{eq}$ is equivalent module of nanotube which can be calculated as follows:

$$
E^{eq} = 2tE^e / r
$$

with $t = 0.34$ nm, $E^e$ is the module of carbon nanotube. $\beta$ can be obtained from the following equation [25]:

Fig. 5. Stick–slip behavior of SWCNT-based composites.
Fig. 6. (a–f) Are the RVE’s first six mode shapes in cantilevered type.
where $A = 2\pi r^2$ is the contact area between nanotubes and matrix material and $v$ is the volume of matrix material and $\varphi$ is volume fraction of nanotubes.

To investigate the loss factor in this paper, a tensile displacement is applied to one side of RVE, and the other side is clamped. Displacement is applied in ramp form so results can be obtained in its sub displacements. The displacement is applied until the nanotube strain and matrix's strain become different. In that certain strain, maximum shear stress occurs. So the highest loss factor occurs in that point.

4. Results and discussions

4.1. Modal analysis

First the natural frequencies of the RVE are obtained in cantilevered case, which one side of the RVE is clamped. The mode shapes of a 10 nm RVE which is contained of a nanocomposite with SWCNT (10, 0) are shown in Fig. 6.

Fig. 7 shows the natural frequencies of 10 mode shapes of a 5 nm RVE.

Fig. 8 indicates that SWCNT in nanocomposites increases natural frequencies compared to the resin.

As Fig. 9 shows increasing in volume fractions cause higher frequencies; this presents the influence of nanotubes in high frequencies. Materials which tremble in higher frequencies achieve to their intensification frequencies later, because the intensification frequencies of them are higher.

Nanotubes different diameter sizes cause different natural frequencies. In consequence of increasing nanotube diameter, an increase in frequencies occurs. This fact occurs in nanocomposites as shown in Fig. 10 in the present RVE.

4.2. Damping results

This model behaves exactly as the concept of stick–slip motion behavior expects and also follows the equations that belong to this concept. From the results of ANSYS finite element models the critical shear stress $\tau_{\text{max}}$ and dissipation energy $U_{\text{diss}}$ were found and used with the model properties values such as radius, area and young modulus to calculate the interfacial damping ratio from the equations of Section 3.2.

The energy dissipation and loss factor for different aspect ratios were investigated by the process introduced above and the results are shown in Fig. 11. For nanoscale materials the simulations are not very accurate but they can display nanocomposites behaviour, as it can be seen, both energy dissipation and damping ratio are increased due to nanocomposite’s aspect ratio increasing.
By considering the stick–slip concept between nanotube and matrix [26], one side of the RVE was clamped and the other side was pulled by applying tensile displacement in axial direction. It was obtained that, up to a specific strain, the nodes of nanotube and corresponded nodes on matrix, have similar displacement, and by increasing the strain, at internal face of matrix and nanotube slip occurs. Because of this the displacement of matrix nodes will be more than corresponded nodes on nanotubes.

From results, as shown in Fig. 12, it is obvious that at the critical strain point, because of the highest friction between nanotube and internal face of matrix, dissipation energy will be maximum, and enhancement in energy dissipation causes maximum loss factor.

Fig. 12 shows the influence of increasing the volume fraction in nanocomposites with SWCNT with critical shear stress 0.95814 MPa.

Table 1 shows the comparison of first two frequencies of this paper’s model in different volume fractions and what Rajoria and Jalili obtained from experimental works [27].

5. Conclusions

Vibrational analysis is used to extract natural frequencies of a cantilevered RVE model. It is observed that the natural frequencies of RVE are greater than pure resin’s. In cantilever boundary conditions type, we can see that the axial vibration frequency of RVE is greater than its bending vibration frequency so its axial stiffness is greater than its bending stiffness; consequently the nanotube reinforced composites have more strength in the direction which is parallel to CNT longitudinal axis. Also, increasing volume fraction causes an increase in natural frequencies which indicates the effect of nanotubes in improving the nanocomposite’s behavior in resonance. Finally, the damping ratio of RVE was obtained from the stick–slip concept in nanocomposites. The results shows that
dissipation energy and loss factor increase for longer RVEs. From results a specific point was found where the RVE has the highest loss factor. It is shown that after this point the loss factor decreases so the influence of nanotube existence in damping characteristics decreases. The relation between loss factor and natural frequencies also shows that high loss factors cause high natural frequencies, this means achieving to natural frequencies which cause resonance to occur later.

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