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Investigate the Buckling Behavior of Beams Made of Carbon Nanotube (CNT)-Reinforced Polymer Matrix Nanocomposites by Finite Element Method

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Abstract

In this study, buckling behavior of beams made of Carbon Nanotube (CNT)-reinforced polymer matrix nanocomposites is investigated. To this end, the mechanical properties including elastic modulus and Poisson's ratio of nanocomposites are extracted based on an analytical micromechanical model. The distribution type of CNTs into the nanocomposite is considered to be random and aligned, and micromechanical formulations of Mori-Tanaka (M-T) method are extracted for these two conditions. The interphase created due to non-bonded van der Waals interactions between the CNT and polymer matrix is incorporated in the simulation of mechanical properties. after calculating the elastic properties, the buckling behavior of nanocomposite beams is studied using the finite element method. The effects of CNT volume fraction, CNT diameter, temperature variation, thickness and adhesion exponent of interphase at micro-scale on the buckling behavior are examined. Also, the dimensions and cross-section type of beams as well as number of elements at macro-scale on the buckling behavior are investigated. The results show that the increase of CNT volume fraction leads to an increase in buckling loads of nanocomposite beams. So, as an important outcome, adding the CNTs into the nanocomposite beams can postpone the induced damage due to buckling. The comparison between the results of the present micromechanical method and experimental data indicates that the model has a reasonable accuracy.

Keywords: Nanocomposite beam, Carbon nanotube, Buckling, Micromechanics.

1 | Introduction

The foundation of structure-property relationships for polymer matrix nanocomposites reinforced with Carbon Nanotubes (CNTs) is a crucial principle for such materials, enabling reliable and optimal designs. Consequently, numerous researchers have reported the thermo-mechanical properties, including Young's

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modulus, tensile strength, and thermoelastic coefficient, of polymer matrix nanocomposites following the addition of CNTs.

In the realm of experimental methods, in 1998, Schadler et al. [1] found that adding 5 wt.% of Multi-Walled Carbon Nanotubes (MWCNTs) to an epoxy matrix could increase the Young's modulus of the nanocomposite by up to 20%. In another experimental study in 2000, Qian et al. [2] observed that incorporating 1 wt.% CNTs into polystyrene (polymer matrix) improved the elastic modulus and tensile strength of the nanocomposite by 36-42% and 25%, respectively. Furthermore, in 2004, Zhou et al. [3] reported that adding 1 to 4 wt.% of CNTs to epoxy polymer would result in a 30 to 70% increase in the mechanical properties of the nanocomposite. In 2006, experimental results by Yeh et al. [4] demonstrated that adding 4 wt.% MWCNTs to phenolic polymer led to a 46.7% and 64.4% increase in the elastic modulus and tensile strength of the nanocomposite, respectively. Additionally, according to experimental reports by Rong et al. [5] in 2010, it was found that the elastic stiffness (elastic modulus) of a Polyetheretherketone (PEEK) matrix nanocomposite with 0.5, 1, 3, and 5 wt.% CNTs was 1088.17, 1122.31, 1269.18, and 1333.1 MPa, respectively, while the elastic stiffness of neat PEEK was 1019.12 MPa. Also, Jia et al. [6] in 2011 conducted experiments on polypropylene matrix nanocomposites and reported that adding only 0.3 vol.% MWCNTs resulted in a 15% increase in Young's modulus.

Shirasu et al. [7] investigated the thermoelastic coefficient of unidirectional CNT-reinforced epoxy matrix nanocomposites. Their results were presented in the temperature range of 30-60 °C for various volume fractions of CNTs. According to experimental observations, the thermoelastic coefficient of the nanocomposite decreases with increasing volume fraction of CNTs. Xu et al. [8] examined the effects of adding CNTs on the thermoelastic properties of Polyvinylidene Fluoride (PVDF) matrix nanocomposites. The thermoelastic coefficient of the nanocomposite was reported for various volume fractions of nanotubes, up to 49%. They also showed that the thermoelastic properties of the polymer matrix nanocomposite improve with increasing volume fraction of nanotubes. Shokrieh et al. [9] fabricated samples of epoxy matrix nanocomposites containing 0.1, 0.5, and 1 wt.% CNTs. According to experimental reports, it was found that the thermoelastic coefficient of the epoxy matrix nanocomposite reinforced with 0.1, 0.5, and 1 wt.% CNTs decreased by 6%, 21%, and 23.7%, respectively, compared to the neat polymer. Kaleemullah et al. [10] also studied the thermoelastic coefficient of polybenzoxazine matrix nanocomposites reinforced with CNTs.

Sabouri and Ayatollahi [11] experimentally investigated the effect of MWCNTs on the fracture resistance of epoxy matrix nanocomposites under out-of-plane shear loading (Mode III fracture) compared to their effect under tensile loading (Mode I fracture). Due to its low viscosity and wide industrial applications, epoxy LY-5052 was used to fabricate the nanocomposite specimens. The considered weight percentages for CNT content in these specimens were 0.1, 0.5, and 1%. In the fabrication process of the nanocomposite samples, the ultrasonication method was employed for homogenizing nanoparticles in the matrix resin. In these tests, a loading fixture for mixed-mode loading was used to measure the fracture resistance of neat epoxy and nanocomposite samples under Mode I and Mode III loading conditions. The obtained results indicate that in both loading modes, increasing CNT content up to 1 wt.% enhances the fracture resistance compared to neat epoxy. However, the maximum Mode I and Mode III fracture toughnesses were obtained for nanocomposites containing 0.5 and 1 wt.% CNTs, respectively. Finally, the observed trends in the experimental results were discussed using the micromechanisms influencing the role of CNTs.

As mentioned, predicting the mechanical properties of polymer nanocomposites reinforced with CNTs is an important principle for their reliable and optimal designs. Conducting diverse experiments, whether destructive or non-destructive, for each mechanical property is highly costly, labor-intensive, time-consuming, and cumbersome. Certainly, performing all of them in practice is impossible due to limitations of testing equipment, difficulties related to nanocomposite fabrication processes, as well as exorbitant costs and time constraints. Furthermore, obtaining comprehensive information regarding each experimental variable is very difficult and practically impossible. Therefore, many researchers have focused their studies on theoretical methods to identify the effective properties of composite materials, aiming both to justify the observations made with experimental data and to extract the required information that is not accessible through experimental methods.

Theoretical studies conducted on composite materials containing CNTs are divided into three major groups: 1) Atomic modeling [12], 2) Multi-scale modeling [13], and 3) Micromechanical modeling [14], [15]. In the domain of analysis, extraction of properties, and optimization of multi-material systems, numerical and analytical micromechanical models are widely used. Micromechanics is the study of the behavior of a nanocomposite material where the effect of interaction between its constituent components at the microscopic scale on the material's properties is considered. The fundamental question of micromechanics is: what relationship exists between the properties of the nanocomposite and the properties of its constituent components, namely the polymer matrix and the reinforcement phase, which is the CNT? In fact, the primary goal of micromechanics is to obtain the macroscopic properties of nanocomposite materials from their constituent microstructures. The inherent characteristics of the constituent structures of the nanocomposite are preserved in the micromechanical method, and its effective properties are determined in terms of the properties of the constituent components, including the CNT and polymer matrix, their volume fraction, and the interaction between these phases, which pertains to the microstructural geometry. Numerous numerical [16] and analytical [17] micromechanical models have been proposed to predict the response of nanocomposite materials under various thermal and mechanical loading conditions. Cylindrical models and unit cell models are two major groups of analytical micromechanical models with simplifying assumptions regarding the geometry of the composite material. The cell method [18] is among the most famous unit cell models. An analytical micromechanical model based on the unit cell method was also presented in [19] to study the behavior of nanocomposite materials reinforced with CNTs. The accuracy of the predictions from these micromechanical models depends on the precise modeling of the phases and their interaction.

Chen and Liu [20] investigated the mechanical properties of polymer matrix nanocomposites containing unidirectional CNTs using a finite element micromechanical method with a square Representative Volume Element (RVE). Elastic moduli and Poisson's ratios in the longitudinal and transverse directions were extracted for various values of CNT volume fraction. The results showed that adding 3.6 vol.% CNTs to the polymer material increased the Young's modulus of the nanocomposite by 33%.

Furthermore, Wan et al. [21], using a finite element micromechanical model, studied the effects of CNT length and the interphase region between the nanotube and resin on the mechanical properties of the nanocomposite. They reported that the reinforcing effect of long nanotubes in the nanocomposite is greater than that of short nanotubes.

Karimi et al. [22] investigated the elastoplastic properties of a polymer matrix nanocomposite, focusing on several micro-scale factors. For this purpose, a combination of the finite element method and micromechanics was used. Considering the imperfect bonding nature between the nanotube and the polymer matrix, a multi-scale finite element approach was employed to replace the nanotube and the interface region with an equivalent solid fiber. Then, using the Mori-Tanaka (M-T) mean-field method, the stress-strain curves of the nanocomposite were extracted. Using these, the influence of nanotube orientation angle on Young's modulus, the effect of nanotube length on elastoplastic properties, and the impact of nanotube agglomeration on elastoplastic behavior were investigated. Examining the nanotube length also revealed that nanotubes with lengths between 10 and 300 nm have a significant effect on the Young's modulus of the nanocomposite, whereas the effect of shorter and longer lengths is not as considerable. Moreover, ignoring agglomeration, increasing the volume fraction of nanotubes leads to an increase in the nanocomposite's stiffness. However, nanotube agglomeration results in a decrease in nanocomposite stiffness. The negative impact of this phenomenon is such that, in some cases, increasing the volume fraction does not increase the stiffness of the nanocomposite but rather decreases it.

Ebtasi and Irani [23] evaluated the factors affecting the mechanical properties and fracture mechanism of polymer nanocomposites reinforced with pristine and functionalized CNT. Modeling was performed at nano and micro scales. The effects of structural defects (voids) and covalent bonds resulting from the functionalization process of nanotubes were investigated at the nano-scale, and the distribution, shape, and curvature of nanotubes were examined at the micro-scale. It was reported that factors such as distribution, waviness, and functionalization of CNTs can lead to either a decrease or an increase in the strength of polymer nanocomposites compared to the neat polymer. Additionally, functionalization of CNTs improves the strength of the polymer nanocomposite and reduces its brittleness. On the other hand, structural defects created during the functionalization process of CNTs cause a decrease in the elastic modulus of the nanocomposite. Furthermore, if the curvature of the reinforcing CNTs in the polymer nanocomposite increases, the beneficial effect of functionalization diminishes significantly, and the properties approach those of nanocomposites reinforced with pristine nanotubes.

Using the finite element micromechanical method, Hammerand et al. [24] approximated the elastic modulus, shear modulus, and Poisson's ratio in longitudinal and transverse directions for straight CNT-reinforced epoxy matrix nanocomposites. CNTs with identical geometric conditions were modeled in two ways: as an equivalent solid nanofiber with transversely isotropic properties, and as a hollow nanotube with isotropic properties. According to reports, the elastic properties of the nanocomposite obtained from the two modeling approaches were found to be very close.

Zhang and He [25], using an analytical concentric cylinder micromechanical model, approximated the longitudinal Young's modulus of CNT-reinforced epoxy matrix nanocomposites. Increasing four factors, including the thickness and elastic modulus of the interphase, the aspect ratio and volume fraction of nanotubes, as well as decreasing the nanotube diameter, leads to an improvement in the nanocomposite's Young's modulus. The results clearly showed that the mechanical properties of the nanocomposite would not be affected by the nanotube aspect ratio if the aspect ratio exceeds 35.

Structural reconstruction from statistical structures is an area of great interest due to its importance in nanocomposite design. A new method was proposed by Mahdavi et al. [26]. In this method, a large number of volume elements are used to reconstruct the nanocomposite structure. Using this method, nanocomposites containing nanotubes can be easily reconstructed using statistical methods, and the reconstructed samples adequately represent their properties and characteristics. They used the Monte Carlo method for reconstruction. By identifying and obtaining statistical correlation functions from images and experimental samples using an algorithm they presented, samples possessing statistical correlation functions similar to experimental ones were reconstructed. Instead of using various images, information regarding the distribution of nanotubes in the polymer matrix—specifically, the coordinates of the start and end points of the cylindrical segments that eventually connect to form the nanotube—is stored. This allows the reconstructed nanocomposite to be used for future work and can easily be employed in studies requiring simulation and extraction of properties of nanotube composites.

In the micromechanical study of the mechanical properties of polymer matrix nanocomposites reinforced with CNTs using a RVE, it is determined that these properties are functions of the constituent properties and geometric parameters. Therefore, Shokrieh et al. [27] considered an RVE consisting of a surrounding polymer matrix and a CNT at the core, shaped as a rectangular cuboid with a square cross-section. The length and thickness of the RVE, the length of the CNT and its two ends, as well as the volume fraction of the CNT, were considered as variable parameters. Thus, the influence of changes in these parameters on the elastic modulus of the RVE, and consequently on the elastic modulus of the nanocomposite, was studied. Accordingly, analytical relations for the elastic modulus of the RVE were derived, and modeling and analysis were also performed using the finite element method. The results show that at a constant volume fraction, changing either the length or width parameters of the RVE, especially its longitudinal elastic modulus, leads to significant changes. Therefore, using the Halpin-Tsai micromechanical relation and the analytical relations extracted in this study, suitable aspect ratios for the RVE based on volume fraction were obtained and proposed.

A three-dimensional analytical micromechanical model based on a unit cell was designed and generalized by Mahmoudi and Vakilifard [28] to extract the mechanical, thermal, and electrical properties of a piezopolymer nanocomposite reinforced with a CNT. The RVE of the piezo-nanocomposite consists of three phases: the CNT reinforcement, the piezopolymer matrix, and the interphase region. The present model considers the CNT as a solid fiber with transversely isotropic behavior and treats the interface between the CNT and matrix, characterized by van der Waals bonding, using equivalent continuum relations as an isotropic medium; both phases are assumed linearly elastic. The matrix is a piezoelectric material that is mechanically isotropic and elastic, polarized perpendicular to the CNT. The arrangement of CNTs in the matrix is assumed to be regular and square. They investigated the effects of volume fraction, aspect ratio of the CNT, and effective thickness of the interphase on the overall properties of the piezo-nanocomposite. The results indicated that even small amounts of CNT volume fraction have a significant effect on improving the nanocomposite's properties. Furthermore, modeling the interphase region significantly impacts most properties of the nanocomposite, thus, its modeling is essential for a more realistic prediction of the nanocomposite's behavior.

Research has also been conducted on the mechanical behavior of structures composed of CNT-containing nanocomposites, including bending, buckling, and vibration analyses. For example, Vodenitcharova and Zhang [29] investigated the bending and buckling of a single-walled CNT-reinforced nanocomposite beam using the Airy stress function. In another study, the buckling of a CNT-reinforced nanocomposite plate under uniaxial compressive load and thermal load was investigated by Shen [30]. He obtained the properties of the nanocomposite plate using a modified rule of mixtures. He also showed that using linearly graded CNTs as a reinforcing phase in nanocomposites increases the critical bending load. Shaat et al. [31] presented a size-dependent bending, buckling, and vibration analysis for Kirchhoff nano-plates based on a modified couple-stress theory considering surface stress effects. They developed an analytical solution for static bending within the couple-stress theory. Torabi et al. [32] studied the thermal buckling of conical shells made of composites reinforced with functionally graded distribution of CNTs. The effective mechanical properties of the nanocomposite material were presented using a modified rule of mixtures. The governing equations were derived based on the first-order shear deformation theory and Donnell's nonlinear strain-displacement relations, using Hamilton's principle. Pre-buckling forces were obtained by considering the membrane solution of equilibrium equations in a linear state. By applying the generalized differential quadrature method in the axial direction and a periodic differential operator in the circumferential direction, the stability equations were discretized, and the critical buckling temperature was calculated. They investigated the effects of various factors, including volume fraction values and distribution type of CNTs, boundary conditions, and geometric parameters, on the thermal buckling of the conical nanocomposite shell. The results showed that volume fraction values and the distribution type of CNTs along the thickness significantly influence the thermal stability of the conical shell made of nanocomposite materials. Mohammadi-Mehr et al. [33] investigated the buckling and free vibration analysis of a nano-composite micro-plate reinforced with various nanotubes resting on an orthotropic elastic foundation based on a sinusoidal shear deformation theory. The properties of the matrix material and reinforcing nanotubes were considered temperature-dependent. By solving the coupled governing equations of motion for the nanocomposite micro-plate, the effects of various factors such as material length scale coefficient, length-to-thickness ratio, length-to-width ratio, orthotropic elastic foundation constants, temperature changes, and volume fraction of reinforcing nanotubes were studied. The research results indicated that increasing the material length scale coefficient, orthotropic elastic foundation constants, the presence of reinforcing carbon and boron nitride nanotubes, and different physical fields not only increase the natural frequencies and critical buckling load of the system but also delay the resonance phenomenon. Malekzadeh and Shojaee [34] also studied the buckling analysis of multi-layered plates reinforced with CNTs. They investigated the effects of nanotube volume fraction, thickness-to-length ratio, different nanotube distributions, and various boundary conditions on the critical buckling load of multi-layered plates. Zhou et al. [35] extended the finite element method for investigating the bending and free vibration of a CNT-reinforced nanocomposite plate. They used a modified rule of mixtures to estimate the properties of the composite plate. In another study, Lei et al. [36] developed a meshless method for analyzing the buckling behavior of a CNT-reinforced nanocomposite plate based on the first-order shear deformation theory. They also employed the modified rule of mixtures in their study. Jafari Mehrabadi et al. [37], using the first-order shear deformation theory, presented the biaxial buckling of a CNT-reinforced nanocomposite plate. They concluded that the critical biaxial buckling load increases with increasing thickness-to-width ratio and CNT volume fraction.

2 | Modeling of CNT-Containing Nanocomposite Beams

One of the most prominent finite element software packages is Abaqus, considered a powerful computer-aided engineering tool for analysis via the finite element method. This software is capable of solving problems ranging from simple linear analyses to the most complex ones. Abaqus possesses a vast library of elements that can model any geometry and, by offering modeling, analysis, and graphical contour and chart presentation capabilities, provides an integrated suite meeting the needs of researchers. Using Abaqus, despite its extensive capabilities, is relatively straightforward. The most complex problems, such as analyzing bridges, shuttles, automobiles, etc., can be easily modeled.

In a simple definition, the finite element method can be divided into four main parts:

I. The first part involves discretizing the domain of interest into numerous smaller regions. The connection points of elements to each other are called nodes, and the collection of elements and their nodes is termed the mesh. Elements can be one-dimensional, two-dimensional, or three-dimensional. Also, depending on the element's dimension, various shapes can be considered for an element. A two-dimensional element can be triangular, quadrilateral, or any other arbitrary shape. Similarly, a three-dimensional element can be tetrahedral, pyramidal, prismatic, or hexahedral.

II. The second part concerns determining the initial approximation for the solution, expressed as a function with unknown constant coefficients, which is usually linear or quadratic. This approximation is established within the domain of a single element and is not applied globally to the entire problem (for example, $U = C_1x + C_2$ is a linear approximation for displacement distribution in a one-dimensional element).

III. The third part involves deriving the system of algebraic equations. In this step, the governing equation is written for each node individually and, after necessary integrations, is transformed into an algebraic equation.

IV. The fourth part involves solving the generated system of equations and subsequently calculating other quantities based on the nodal values.

The structure of interest in this thesis is a beam made of a nanocomposite material containing CNTs. The length of this beam is one meter, and its cross-section is 0.1 m × 0.1 m (100 mm × 100 mm). *Fig. 1* shows a schematic of the beam in two views.

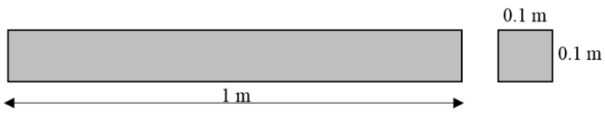


Fig. 1. A schematic of the beam in two views.

The beam modeled in the Abaqus software is shown in *Fig. 2*. Note that the modeling performed in the Abaqus software has been carried out in Three Dimensions (3D).

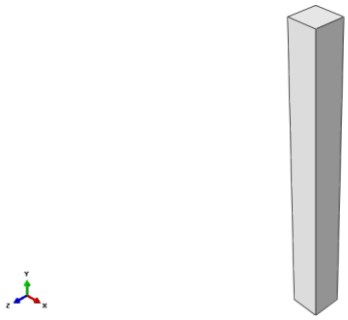


Fig. 2. The beam modeled in the Abaqus software.

The boundary conditions considered for the beam are such that at its end, both translation and rotation are restrained. In other words, a clamped (fixed) condition is applied to it. Furthermore, the loading is applied as a unit pressure on its initial surface. The boundary conditions and loading are shown in *Fig. 3*.

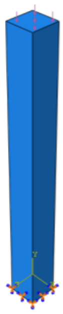


Fig. 3. The boundary conditions and loading applied to the beam.

For meshing the nanocomposite beam, the C3D20 element (a 20-node quadratic brick element) is employed. The element size is set to 0.01 m. The meshed beam is shown in *Fig. 4*. This element size has been selected such that the results do not exhibit a significant dependence on the mesh dimensions, indicating a convergent trend.

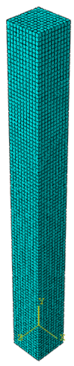


Fig. 4. The meshing of the nanocomposite beam.

It should be noted that the mechanical properties are assigned to the beam using the M–T method. Finally, after meshing the structure, a buckling analysis is performed.

2.1 | Results of Mechanical Properties

In this section, first, to validate the presented micromechanical method, a comparison is made between the model predictions and experimental data as well as other micromechanical approaches. Subsequently, the effects of volume fraction, distribution type of nanotubes, temperature, and also the interphase (including its material and thickness) on the mechanical properties of the nanocomposite are investigated.

3 | Validation of the Micromechanical Model

The validations performed in this thesis consist of two parts: comparisons with other micromechanical models and also with experimental results for various types of polymer matrix nanocomposites reinforced with CNTs.

Initially, a comparison is made between the results of the M–T micromechanical method and the Eshelby method as reported in [38]. This comparison pertains to an epoxy matrix nanocomposite reinforced with randomly dispersed CNTs. The elastic modulus of the CNT and the polymer matrix are 1000 GPa and 3 GPa, respectively. Poisson's ratio for both materials is 0.3. *Fig. 5* illustrates this comparison. In this figure, the normalized elastic modulus of the nanocomposite with respect to the matrix elastic modulus is plotted against the volume fraction of CNTs. The nanocomposite modulus is denoted by E and the matrix modulus by Em. At first glance, it is evident that there is good agreement between the two methods, indicating the appropriate accuracy of the M–T model. From *Fig. 5*, it can be observed that increasing the volume fraction of CNTs leads to an increase in the elastic stiffness of the nanocomposite. In other words, by increasing the amount of CNTs, improved properties can be achieved. This is because the mechanical properties (including elastic modulus) of CNTs are higher than those of the polymer.

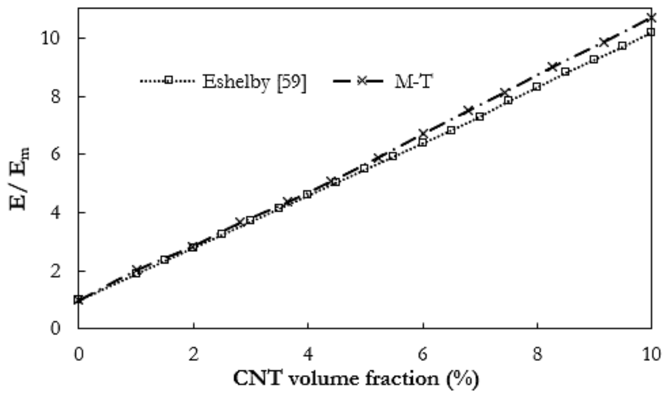


Fig. 5. Comparison between the M–T and Eshelby methods for the elastic modulus of the nanocomposite [38].

Now, the M–T micromechanical model is validated against experimental data on the mechanical properties of an epoxy matrix nanocomposite containing CNTs. Shirasu et al. [39] experimentally investigated the longitudinal elastic modulus of unidirectional CNT-reinforced epoxy matrix nanocomposites. The properties of the CNTs and the epoxy matrix are given in *Table 1*. In this table, E_L and E_T denote the elastic moduli in the longitudinal and transverse directions, respectively. Likewise, v_L and v_T are the Poisson's ratios in the longitudinal and transverse directions, respectively. The average diameter of the CNTs is 39 nm. Furthermore, the interphase thickness and its adhesion parameter are taken as 8 nm and 15.3, respectively. *Fig. 6* presents a comparison of the longitudinal elastic modulus of the unidirectional CNT-reinforced epoxy matrix nanocomposite obtained from the M–T method and from experiments. Overall, the results show that the elastic modulus predicted by the present micromechanical model is very close to the experimental data. It is also observed that a linear increase in the longitudinal elastic modulus of the nanocomposite occurs with increasing volume fraction of CNTs.

Table 1. Mechanical properties of CNTs and epoxy resin.

Material	E_L (GPa)	E_T (GPa)	v_L	v_T
CNT/Epoxy	240	50	0.162	0.47
	2.5	2.5	0.34	0.34

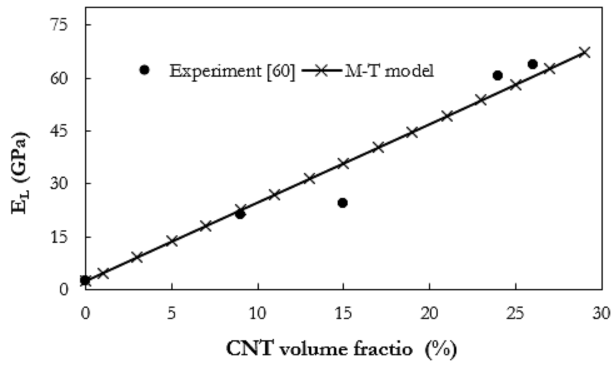


Fig. 6. Comparison between the M–T method and experimental results for the elastic modulus of an epoxy matrix nanocomposite reinforced with aligned CNTs [39].

Another comparison is made between the M–T micromechanical method, which is employed in this thesis, and the Simplified Unit Cell (SUC) micromechanical method. This comparison is presented for the longitudinal elastic modulus of a shape memory polymer matrix nanocomposite reinforced with aligned CNTs. The elastic modulus and Poisson's ratio of the polymer matrix are 0.622 GPa and 0.3, respectively. *Fig. 7* shows the comparison between these two micromechanical models. It is evident that there is acceptable agreement between the two methods. The results also confirm that increasing the amount of CNTs leads to an increase in the elastic modulus of the nanocomposite.

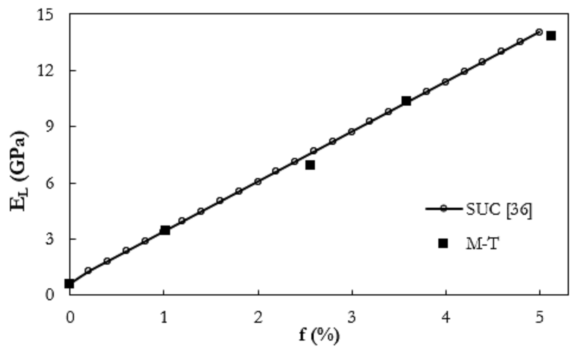


Fig. 7. Comparison between the M–T method and the unit cell method for the elastic modulus of the nanocomposite [19].

Another comparison is made between the results of the M–T micromechanical method and the experimental data [6] concerning the mechanical properties of a polypropylene matrix nanocomposite containing CNTs. The nanotubes are randomly dispersed within the polymer matrix. The mechanical properties of the CNTs are given in *Table 2*. Furthermore, the elastic modulus and Poisson's ratio of polypropylene are 1.85 GPa and 0.45, respectively. Note that the CNTs are considered as a transversely isotropic material, while the polymer matrix is treated as an isotropic material. The average diameter of the CNTs is 50 nm. Moreover, the interphase thickness and its adhesion parameter are taken as 2.38 nm and 23.28 in *Eq. (1)*, respectively. *Fig. 8* presents a comparison of the elastic modulus of the polypropylene matrix nanocomposite obtained from the M–T method and from experiments. It is evident that the results of the present micromechanical model exhibit acceptable accuracy when compared to the experimental data. *Fig. 8* shows that increasing the volume fraction of CNTs within the polymer matrix leads to an increase in the elastic modulus of the nanocomposite.

Table 2. Mechanical properties of CNTs and epoxy resin.

Material	E_L (GPa)	E_T (GPa)	v_L	v_T
CNT	800	49	0.16	0.45

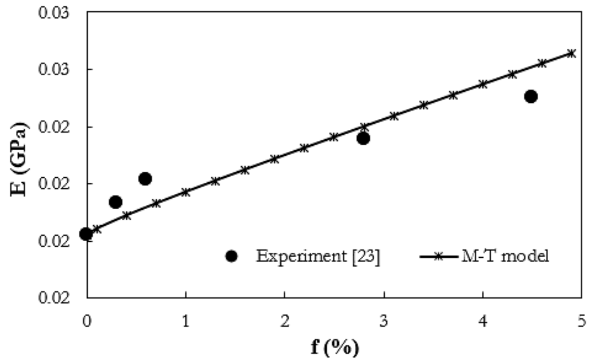


Fig. 8. Comparison between the M–T method and experimental results for the elastic modulus of a polypropylene matrix nanocomposite reinforced with randomly dispersed CNTs [6].

From the overall comparisons made in *Figs. 5-8*, it can be confirmed that the proposed micromechanical model possesses acceptable accuracy. Therefore, it is suitable for extracting the mechanical properties of nanocomposites.

4 | Parametric Studies of Mechanical Properties

In this section, we perform parametric studies and extract the properties of the nanocomposite. For this purpose, the mechanical properties of an epoxy-based shape-memory polymer matrix nanocomposite reinforced with CNTs are extracted. To account for temperature effects, the elastic modulus of the polymer matrix is given according to the following relation [40]:

$$E_P = \frac{1}{\frac{\varphi_f}{E_i} + \frac{1-\varphi_f}{E_e}}, \tag{1}$$

where, in this relation, φ_f and E_e are given as follows.

$$E_e = kT, \qquad \varphi_f = 1 - \frac{1}{1 + c_f(T_h - T)^n}, \tag{2}$$

where T is the temperature of interest, and the remaining parameters in *Eqs. (1)* and *(2)* are provided in *Table 3*. From *Eq. (1)*, it is evident that the elastic modulus of the polymer matrix is temperature-dependent, whereas its Poisson's ratio is constant and equal to 0.3, as per *Table 3*. In addition, the mechanical properties of the (10, 10) single-walled CNT are given in *Table 4* [41].

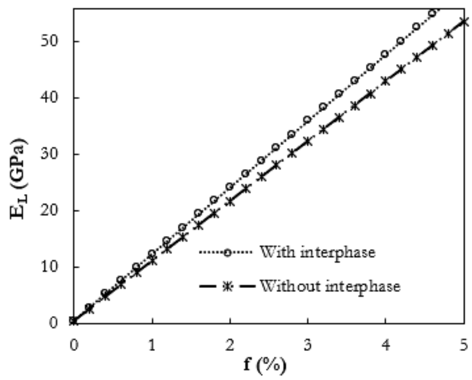
Table 3. Properties of the shape-memory polymer matrix used for parametric studies [40].

c_f (K^{-4})	T_h (K)	E_i (MPa)	k (MPa/K)	n	v
2.76×10^{-5}	358	813	2.64×10^{-2}	4	0.3

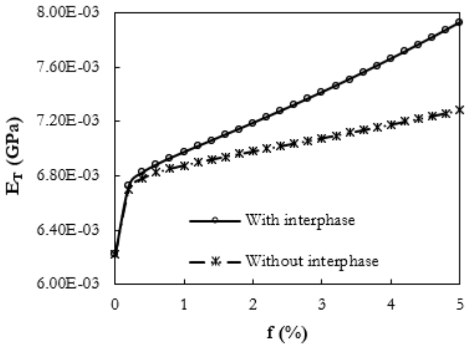
Table 4. Mechanical properties of the (10, 10) single-walled CNT.

E_L (GPa)	G_L (GPa)	v_L	E_T (GPa)	G_T (GPa)
1060	442	0.162	50	17

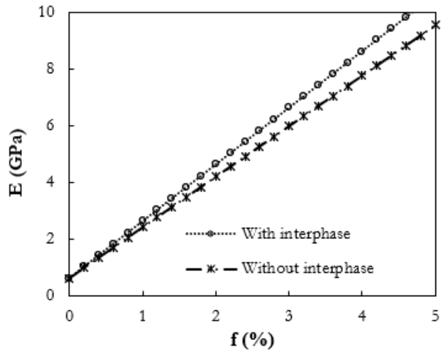
Figs. 9.a and *9.b* show the variations of the longitudinal and transverse elastic moduli, respectively, of the shape-memory polymer matrix nanocomposite reinforced with aligned CNTs as a function of nanotube volume fraction. Furthermore, *Fig. 9.c* presents the elastic modulus of the shape-memory polymer matrix nanocomposite containing randomly dispersed CNTs versus nanotube volume fraction. In these figures, the effects of considering and neglecting the interphase on the elastic properties of the nanocomposite have been investigated. In other words, the results of the M–T micromechanical method have been extracted both with and without the interphase between the nanotube and the polymer. It is observed that increasing the volume fraction of CNTs within the polymer matrix leads to a linear increase in the elastic modulus of both the nanocomposite reinforced with aligned nanotubes and the nanocomposite reinforced with randomly distributed nanotubes.



a.



b.

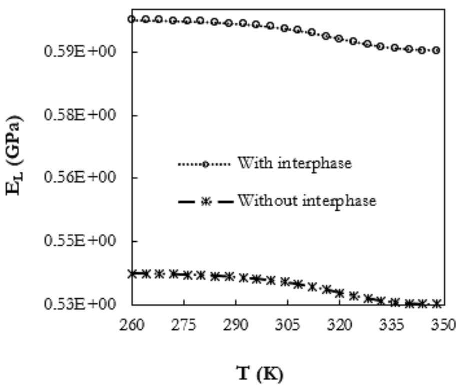


c.

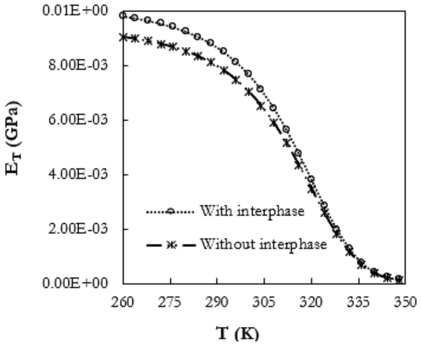
Fig. 9. a. Longitudinal and b. Transverse elastic moduli of the shape-memory polymer matrix nanocomposite reinforced with aligned CNTs versus CNTs volume fraction, and c. Elastic modulus of the shape-memory polymer matrix nanocomposite containing randomly dispersed CNTs versus CNT volume fraction.

However, as shown in *Fig. 9.b*, with increasing volume fraction of CNTs, a nonlinear increase is observed in the transverse elastic modulus of the shape-memory polymer matrix nanocomposite reinforced with aligned CNTs. On the other hand, as can be seen from the results in *Fig. 9*, the elastic modulus of the nanocomposite when the interphase is considered is higher than when the interphase is not included in the modeling. This is because the mechanical properties of the interphase are superior to those of the polymer matrix. In fact, the interphase properties are a function of the properties of both the CNT and the polymer matrix. Therefore, it is expected that the mechanical properties of the interphase lie between those of the nanotube (higher) and those of the polymer matrix (lower). The results also clearly demonstrate that the transverse elastic modulus of the nanocomposite reinforced with aligned nanotubes is the most significantly affected by the presence of the interphase.

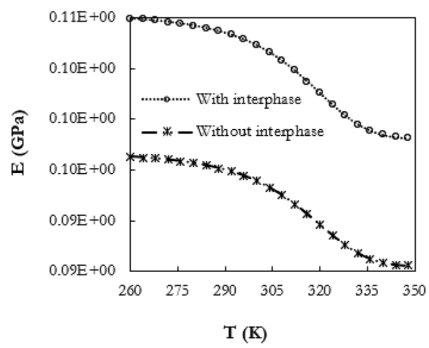
Figs. 10.a and *10.b* show the variations of the longitudinal and transverse elastic moduli, respectively, of the shape-memory polymer matrix nanocomposite reinforced with aligned CNTs as a function of temperature. *Fig. 10.c* also presents the elastic modulus of the shape-memory polymer matrix nanocomposite containing randomly dispersed CNTs versus temperature. The temperature range considered is from 260 K to 350 K. Furthermore, *Fig. 10* illustrates the effects of the interphase formed between the nanotube and the polymer matrix on the elastic stiffness of the nanocomposite. The modeling results reveal that the elastic modulus of the nanocomposite decreases with increasing temperature. As shown in *Fig. 10.a*, this reduction is very slight for the longitudinal elastic modulus of the aligned nanotube-reinforced nanocomposite, whereas, according to *Fig. 10.b*, the decrease is quite significant for the transverse case. The reason for the decrease in the elastic modulus of the nanocomposite with increasing temperature is that the elastic modulus of the polymer matrix decreases with temperature.



a.



b.

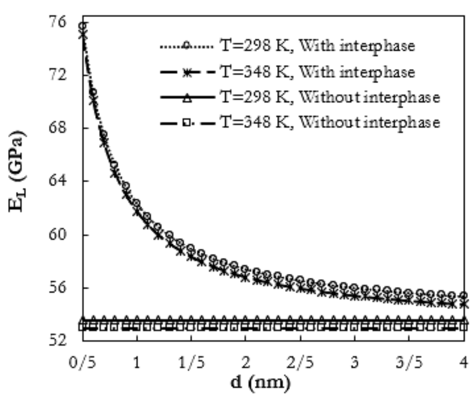


c.

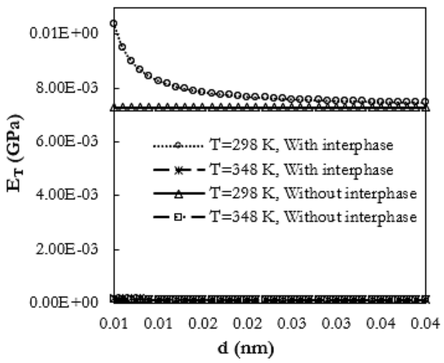
Fig. 10. a. Longitudinal and b. transverse elastic moduli of the shape-memory polymer matrix nanocomposite reinforced with aligned CNTs versus temperature, and c. elastic modulus of the shape-memory polymer matrix nanocomposite containing randomly dispersed CNTs versus temperature.

From *Fig. 10*, it is observed that the mechanical properties of the nanocomposite, when the interphase is considered, are higher than those obtained without the interphase.

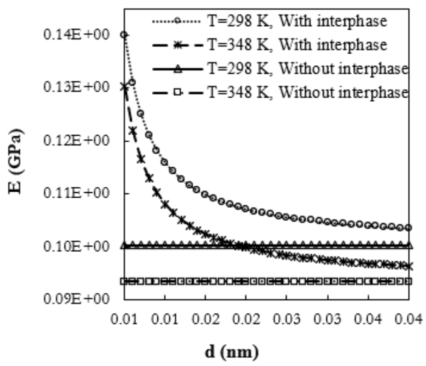
Now, using the M–T micromechanical model, a parametric analysis is presented to study the effects of CNT diameter on the Young's modulus of the shape-memory polymer matrix nanocomposite. *Figs. 11.a* and *11.b* show the variations of the longitudinal and transverse elastic moduli, respectively, of the shape-memory polymer matrix nanocomposite reinforced with aligned CNTs as a function of nanotube diameter. *Fig. 11.c* also presents the elastic modulus of the shape-memory polymer matrix nanocomposite containing randomly dispersed CNTs versus nanotube diameter. The nanotube diameter is varied between 0.5 and 4 nm. Furthermore, in *Fig. 11*, two important parameters, namely temperature and the interphase, have been investigated for their effects on the elastic stiffness of the nanocomposite. The results are obtained at two temperatures: 298 K and 348 K. From the results presented in *Fig. 11*, it can be clearly seen that, in the presence of the interphase, decreasing the nanotube diameter leads to a significant improvement in the mechanical properties of the nanocomposite. The reason for this is that with a decrease in CNT diameter, the surface-to-volume ratio of the nanotubes increases, thereby increasing the volume fraction of the interphase region, which possesses superior mechanical properties compared to the polymer matrix. Consequently, the overall properties of the nanocomposite are enhanced. As can be observed from *Fig. 11*, when the interphase is not considered, variations in CNTs diameter have no effect on the effective stiffness of the nanocomposite.



a.



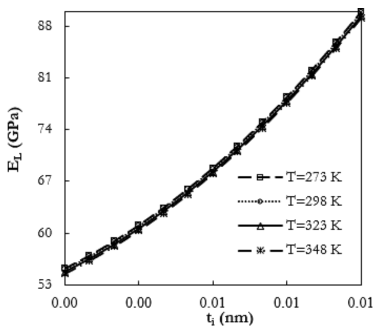
b.



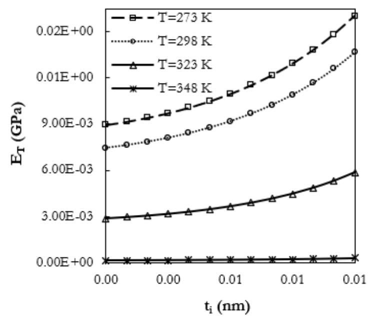
c.

Fig. 11. a. Longitudinal and b. Transverse elastic moduli of the shape-memory polymer matrix nanocomposite reinforced with aligned CNTs versus CNTs diameter, and c. elastic modulus of the shape-memory polymer matrix nanocomposite containing randomly dispersed CNTs versus CNT diameter.

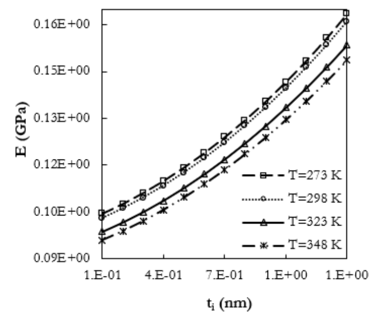
As can be inferred from the above results, the interphase has a significant influence on the mechanical properties of the nanocomposite. Therefore, it is necessary to investigate the effects of its parameters on the elastic stiffness of the nanocomposite. *Figs. 12.a* and *12.b* show the variations of the longitudinal and transverse elastic moduli, respectively, of the shape-memory polymer matrix nanocomposite reinforced with aligned CNTs as a function of interphase thickness (t_i). *Fig. 12.c* also presents the elastic modulus of the shape-memory polymer matrix nanocomposite containing randomly dispersed CNTs versus interphase thickness. The interphase thickness is varied between 0.1 and 1.3 nm. The numerical results have been extracted at four different temperatures: 273 K, 298 K, 323 K, and 348 K.



a.



b.



c.

Fig. 12. A. Longitudinal and b. Transverse elastic moduli of the shape-memory polymer matrix nanocomposite reinforced with aligned CNTs versus interphase thickness, and c. elastic modulus of the shape-memory polymer matrix nanocomposite containing randomly dispersed CNTs versus interphase thickness.

5 | Conclusion

Reinforcing polymer matrix nanocomposites with CNTs is one of the novel methods for enhancing the mechanical properties of these materials for use in advanced industries, including aerospace. Owing to the exceptional properties of CNTs—such as ultra-high stiffness and strength, low coefficient of thermal expansion, and low density—these nanocomposites exhibit significantly superior mechanical properties compared to conventional composites.

To analyze the mechanical behavior of structures made of CNT-reinforced nanocomposites, the effective properties of the material must first be determined. Therefore, in this thesis, the analytical M–T micromechanical model was first presented to extract the mechanical properties of CNT-reinforced nanocomposites. CNTs were initially modeled as aligned fibers, and subsequently, isotropic properties, including elastic modulus and Poisson's ratio, were extracted using appropriate transformation rules. An equivalent solid continuum medium, termed the interphase, was used to describe the van der Waals interaction between the nanotube atoms and the polymer in the micromechanical modeling. Then, the buckling behavior of nanocomposite beams was investigated using the finite element method. For meshing the nanocomposite beam, the C3D20 element (a 20-node quadratic brick element) was employed.

Several comparisons were made between the predictions of the micromechanical model and experimental data. It was determined that the present model can accurately predict the experimental results. The effects of various parameters, including CNT volume fraction and diameter, temperature, and interphase thickness and adhesion parameter, on the longitudinal and transverse elastic moduli, as well as the isotropic elastic modulus, were investigated. In general, increasing the volume fraction of CNTs leads to an increase in the Young's modulus of the nanocomposite. It was found that increasing the CNT volume fraction results in a nonlinear increase in the transverse elastic modulus of the shape-memory polymer matrix nanocomposite reinforced with aligned nanotubes. Furthermore, decreasing the CNT diameter led to improvements in mechanical properties due to the increased interphase content within the nanocomposite. Without considering the interphase, changes in CNT length had no effect on the effective stiffness of the nanocomposite. Increasing the interphase thickness improved the elastic properties of the nanocomposite. This is because an increase in interphase thickness raises the volume fraction of this component, thereby amplifying its influence on the overall properties.

The results of the mechanical behavior analysis showed that increasing the volume fraction of CNTs enhances the buckling load for a beam made of the nanocomposite material. Therefore, as a very important conclusion, adding CNTs to the beam can significantly delay failure due to buckling. The results also indicated that increasing temperature reduces the buckling load for the nanocomposite beam, which is attributed to the decrease in stiffness of the nanocomposite material with rising temperature. Additionally, the finite element analysis of the nanocomposite structure revealed that the buckling load for a solid square cross-section nanocomposite beam is higher than that for a hollow square cross-section nanocomposite beam up to the fourth buckling mode. However, in the fifth mode, the buckling load for the hollow square cross-section nanocomposite beam exceeds that of the solid square cross-section nanocomposite beam.

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