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The Structural Buckling of Carbon Nanotube-Reinforced Nanocomposite

Hossein Masoomi*

Department of Civil Engineering, Science and Research Branch, Islamic Azad University, Tehran; civil_1363@yahoo.com.

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Abstract

The recent developments of lightweight and highly-strong structural materials have resulted in the increased attention paid to the nanocomposites reinforced with Carbon Nanotubes (CNTs), owing to their unique mechanical properties. This paper explores the stability analysis of the nanocomposite beams reinforced with CNTs via a computational model based on the finite element method. The properties of the nanocomposite material are determined with the help of the Mori-Tanaka micromechanical approach where various types of CNT dispersion, such as aligned and random distribution, are taken into account. Moreover, the effects of weak Van der Waals interaction in the CNT-matrix interface are taken into consideration. The influence of some important design parameters like the volume fraction of CNT, diameter of nanotubes, thermal condition, interfacial interphase thickness, and geometry of the beam cross-section is examined regarding the influence of these parameters on the critical buckling capacity. The results reveal that increasing the volume fraction of CNT significantly enhances the stiffness of the material, making it highly resistant to elastic instability. Additionally, the presence of the interfacial interphase layer plays a significant role in improving the performance of the structure. It is concluded from the numerical analysis that the temperature rise has a negative impact on the buckling behavior since the effective stiffness of the nanocomposites decreases. In addition, it has been found out that the utilization of CNTs with small diameters and larger interphase thickness leads to higher critical buckling loads especially by considering the interface phenomena. Moreover, it is noted that the beam geometry has a great influence on stability behavior. Thus, the longer beams have lower buckling loads, while the increased cross-sections lead to the improvement of the load-carrying capacity. In addition, it can be stated that the beams with hollow cross-sections have better performance than beams with solid cross-sections. From the mesh analysis, it is shown that there is no significant change in the results after reaching an appropriate number of elements. Therefore, computational cost efficiency can be achieved without losing accuracy.

Keywords: Buckling behavior, CNT-reinforced nanocomposite beams, Finite element modeling, Mori–tanaka homogenization method.

1 | Introduction

The evolution of materials science has been greatly affected by the appearance of nanotechnology, which created a new set of opportunities for engineering and controlling materials at very small dimensions. The possibilities for controlling atoms and molecules and the idea of a nanomachine have been discussed by

Corresponding Author: civil_1363@yahoo.com

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Feynman [1] and became a basis for the further development of nanoscale technology [2]. Though the practical implementation of these ideas needed several decades of development, they played an important role in the field of nanoscience.

At present, nanotechnology can be regarded as the science and engineering of materials, devices and structures at dimensions smaller than 100 nanometers. Due to the significant increase in the effect of surface phenomena, quantum effects and interactions between atoms, materials demonstrate unusual behavior and properties. This makes it possible to create new types of advanced materials possessing certain mechanical, electrical, optical, chemical, or biological properties, which cannot be attained by other means [3].

Nanotechnology is not just about reducing material sizes; it aims to modify the matter in such a way that it could demonstrate better performance depending on the purpose. With increasing knowledge about nano effects, a variety of new materials and technologies was developed that provided solutions for problems encountered by scientists and industries. Unique characteristics of nanostructured materials have been used for advancement in such fields as biomedical engineering, energy conversion and storage, electronics, environmental technologies, and new structural materials [4].

Thanks to its ability to increase material capabilities and provide the opportunity to develop next generation systems, nanotechnology is one of the key technologies related to the ongoing fourth industrial revolution. Implementation of nanoscale materials in engineering provides possibilities to develop light, strong and efficient structures with improved characteristics [5]. Special importance is given to the development of multifunctional materials possessing enhanced mechanical strength, electrical conductivity, thermal stability and other useful properties.

Nanotechnology is often regarded as a modern scientific field; nevertheless, there are ancient technologies where nanoscale effects were employed. Ancient people used nanoparticles by accident while developing their technological products; Roman craftsmen manufactured colorful glasses with the help of nanoparticles of metals already in the fourth century A.D. Nevertheless, this technology was not grounded on scientific knowledge. It became possible to systematically study materials with nanoscale structures due to the development of quantum mechanics, microscopy and modern materials science.

Nanotechnology can be viewed as a multidisciplinary field uniting physics, chemistry, biology and engineering. With the help of nanotechnology, scientists have been able to work with the structure of materials on an extremely precise level, which results in constant improvement in the development of functional materials. Nanostructured materials include different types of materials, but carbon-based nanomaterials, especially Carbon Nanotubes (CVTs), have gained special popularity due to their unique physical and mechanical properties.

1.1 | Nanomaterials and Their Significance

Nanomaterials represent the fundamental components of nanotechnology and have attracted considerable attention due to their distinctive characteristics arising from their nanoscale dimensions. These materials generally contain structural features with at least one dimension below 100 nanometers, where size-dependent phenomena significantly influence their overall behavior. Unlike conventional bulk materials, nanostructures possess a remarkably high surface-area-to-volume ratio, causing a greater proportion of atoms to exist at or near the surface. As a result, surface interactions become dominant and can substantially modify mechanical strength, chemical activity, electrical conductivity, and other functional properties [3].

The exceptional performance of nanomaterials is mainly associated with the combination of nanoscale size effects, enhanced surface interactions, and quantum mechanical phenomena. When material dimensions are reduced to the nanometer range, classical theories are often insufficient to describe their behavior, as atomic arrangements and electron confinement effects begin to play a critical role. These nanoscale characteristics provide opportunities for engineering materials with improved performance and customized functionalities for specific applications.

Based on their structural geometry and dimensionality, nanomaterials can be categorized into four major groups. Zero-Dimensional (0D) nanomaterials, including nanoparticles and quantum dots, exhibit nanoscale dimensions in all directions and are widely employed in applications such as optical devices, imaging technologies, and biomedical systems. One-Dimensional (1D) nanostructures, including nanowires and nanotubes, possess nanoscale dimensions in two directions while extending along a third direction, making them highly suitable for electronic, sensing, and reinforcement applications. Two-Dimensional (2D) nanomaterials, such as graphene sheets and nanofilms, have atomic-scale thickness with extended surface dimensions and are considered promising materials for flexible electronics, energy storage devices, and advanced sensors. Three-Dimensional (3D) nanostructured materials are generally produced by assembling nanoscale building blocks into bulk structures, enabling the development of materials with enhanced mechanical and functional properties [6], [7].

The fabrication of nanomaterials can be achieved through two primary strategies: Top-down and bottom-up manufacturing techniques. The top-down approach involves the reduction of larger structures into nanoscale components using physical processes such as mechanical milling, lithography, or etching. Although this method is relatively straightforward, controlling defects and achieving precise nanoscale architectures can be challenging. In contrast, the bottom-up strategy involves the controlled assembly of atoms or molecules to construct nanostructures with desired characteristics. Due to its ability to provide better structural control, this approach has become widely used for synthesizing advanced nanomaterials, including CNTs, nanowires, and quantum dots [8], [9].

One of the most important advantages of nanomaterials originates from their increased active surface area. The large number of available surface atoms enhances interactions with surrounding environments, resulting in improved catalytic activity, chemical sensitivity, and electrical performance. These features have enabled the integration of nanomaterials into numerous high-performance technologies, including structural composites, renewable energy systems, electronic components, and biomedical devices [10]. For instance, nanoparticles can significantly improve catalytic processes by providing a greater number of active sites, thereby increasing the efficiency of chemical reactions in applications such as fuel cells, hydrogen production, and environmental purification systems [11].

In addition to surface-related effects, quantum phenomena contribute significantly to the unique behavior of nanoscale materials. As the dimensions of a material approach atomic scales, electrons become spatially confined, leading to modifications in optical and electronic characteristics. Quantum confinement is a notable example of this effect, where the properties of semiconductor nanoparticles become dependent on their size. Quantum dots, which are nanoscale semiconductor crystals, exhibit tunable optical responses due to size-dependent energy levels, making them valuable for applications such as biological imaging, light-emitting devices, and advanced display technologies [12].

Overall, nanomaterials provide a versatile platform for the development of next-generation engineering systems due to their ability to combine superior mechanical, electrical, thermal, and chemical properties. Among the various classes of nanomaterials, carbon-based structures—particularly CNTs—have emerged as highly promising reinforcement materials because of their exceptional strength, stiffness, and multifunctional characteristics.

1.2 | Applications and Advancements

CNTs are among the most extensively studied and utilized nanomaterials. Discovered in 1991 by Iijima [13], these hollow cylindrical structures made of rolled graphene sheets possess remarkable electrical, mechanical, and thermal properties. CNTs exist in two main forms: Single-Walled Carbon Nano Tubes (SWCNTs) and Multi-Walled Carbon Nano Tubes (MWCNTs). Both types have found applications across various industries, from electronics to aerospace, due to their exceptional strength, electrical conductivity, and low density [14]. Mechanical properties make CNTs ideal for reinforcing materials in composites. Their tensile strength ranges from 13 to 52 gigapascals, making them far stronger than conventional materials like steel. Combined with their low density, this strength enables the production of lightweight, durable materials with high impact resistance. This property is precious in the automotive, aerospace, and defense industries, where material weight and durability are crucial factors. In addition to their mechanical properties, CNTs exhibit unparalleled electrical conductivity. Their conductivity is thousands of times better than copper's, making them excellent candidates for use in advanced electronics, including transistors, sensors, and integrated circuits. CNTs are suitable for thermal management applications in electrical systems where effective heat dissipation is crucial, given that their thermal conductivity is twice that of diamond [15]. Reinforcing polymer-based nanocomposites represents one of the most promising applications for CNTs. Researchers have enhanced the mechanical, electrical, and thermal properties of polymers by incorporating a small volume fraction of CNTs, enabling their use in high-performance applications. For example, adding just 1% by weight of CNTs to a polymer matrix can significantly increase the composite's strength and stiffness. This enhancement has been demonstrated in various studies, where the addition of CNTs to materials like epoxy and polypropylene has improved properties, such as Young's modulus and tensile strength. CNTs are also being used in energy storage systems, such as lithium-ion batteries and supercapacitors, where their high surface area and conductivity can enhance energy storage capacity and efficiency. In solar cells, CNTs improve the charge transport properties, increasing the overall efficiency of photovoltaic devices. Their use in hydrogen storage applications has also shown promising results, particularly in fuel cell technology [16]. The biomedical field has also seen significant advancements through the use of CNTs. The ability to penetrate cells has made these agents valuable in drug-delivery systems, allowing for the rapid transport of therapeutic compounds to specific cells or tissues. Furthermore, CNTs are being explored in biosensors, where their electrical properties can detect minute changes in biological environments, such as the presence of certain biomolecules or changes in pH. CNTs have a unique structure composed of carbon atoms bonded in a hexagonal mesh, which results in remarkable mechanical properties. SWCNTs consist of a tubular shell of graphene sheets, while MWCNTs comprise several concentric cylinders of graphene layers. This structural variation results in differences in strength, with small-diameter, near-armchair nanotubes demonstrating the highest tensile strengths because of their specific structure-dependent stress distribution [17]. The sp2 carbon bonds in CNTs provide a tensile strength that surpasses both steel and Kevlar, making them even stronger than the sp3 bonds found in diamonds. CNTs are available in various forms, including coated, dispersed, and functionalized versions, allowing for versatile applications. However, their strength depends on factors like chirality, with structural defects influencing their ultimate performance in composites [17]. CNT-reinforced polymer nanocomposites hold significant potential in various fields, including aerospace, biomedical devices, and automotive applications, due to their high specific strength, lightweight, and excellent stiffness properties [18–20]. Since Iijima's discovery in 1991 [13], there has been a growing interest in leveraging CNTs in polymers to overcome the limitations of natural fiber-reinforced composites. While natural fillers offer advantages like biodegradability and ecological benefits [21], [22], The TBL framework emphasizes the importance of economic, social, and environmental considerations in manufacturing processes. While there have been numerous studies on synthetic rubber nanocomposites, there is limited research on the biomedical applications of Natural Rubber (NR) reinforced with CNTs. This review aims to bridge that gap by exploring the potential of CNT/NR nanocomposites for in-vitro biomedical purposes, advocating for sustainability in their development as a future trend in the literature. Nanotechnology, particularly through the development of nanomaterials like CNTs, is transforming industries by enabling the production of materials with superior properties. From quantum dots that revolutionize medical imaging to CNT-reinforced composites that enhance mechanical and electrical performance, nanotechnology applications continue to expand. As researchers further explore the properties of nanomaterials and develop new synthesis methods, the potential for future innovations in energy, medicine, and materials science remains boundless. The primary objective of this study is to analyze the buckling behavior of CNT-reinforced nanocomposite beams using the FEM. By incorporating CNTs into polymer-based nanocomposites, this research aims to understand how these reinforcements affect the mechanical properties, particularly under compressive loads that lead to buckling. The study utilizes the M-T micromechanical model to determine fundamental mechanical properties, such as the elastic modulus and Poisson's ratio, for both aligned and randomly distributed CNT configurations. To more accurately capture the behavior of the nanocomposite material, non-bonded van der Waals interactions between the CNTs and the polymer matrix are incorporated into the model. This research contributes significantly to the field by providing a comprehensive simulation of the buckling behavior in CNT-reinforced nanocomposite beams through FEM simulations in Abaqus. It explores various factors—including CNT volume fraction, nanotube diameter, temperature changes, and beam thickness—to assess their impact on the critical buckling load. Second, the study offers a robust framework for determining the elastic properties of these nanocomposites, utilizing the M-T model to account for both aligned and random CNT orientations. Third, the research explores the effects of factors like cross-sectional dimensions and the number of macroscopic elements on buckling behavior, offering insights into optimizing the design of CNT-reinforced structures for enhanced stability. Finally, the study compares its simulation results with experimental data, validating the accuracy of its models and providing a foundation for future advancements in developing high-performance nanocomposite materials.

2 | Methodology

2.1 | Mechanical Properties

Among the various nanostructured materials developed during the advancement of nanotechnology, CNTs have emerged as one of the most remarkable and extensively investigated nanomaterials. Since their discovery by Iijima in 1991 [13], CNTs have attracted significant scientific and industrial interest because of their exceptional combination of mechanical strength, electrical conductivity, thermal stability, and extremely low density [14]. These unique characteristics have positioned CNTs as highly effective reinforcement agents for the development of advanced composite materials with superior multifunctional performance.

Structurally, CNTs consist of cylindrical graphene layers formed by rolling one or more sheets of carbon atoms arranged in a hexagonal lattice. Based on the number of graphene walls, CNTs are generally classified into two main categories: SWCNTs, which contain a single graphene cylinder, and MWCNTs, which consist of multiple concentric graphene layers. The structural configuration, chirality, diameter, and number of walls strongly influence the physical and mechanical behavior of CNTs, resulting in a wide range of properties suitable for different engineering applications [14].

The outstanding mechanical performance of CNTs has made them attractive candidates for reinforcing polymer-based materials. Their exceptional tensile strength, which can reach values in the range of several tens of gigapascals, combined with their nanoscale weight, provides composites with remarkable specific strength and stiffness. Compared with conventional engineering materials such as steel, CNTs offer significantly higher strength-to-weight ratios, making them particularly suitable for applications where weight reduction and structural reliability are critical requirements. Consequently, CNT-reinforced materials have received considerable attention in aerospace, automotive, defense, and other advanced structural applications.

Beyond their mechanical advantages, CNTs possess extraordinary electrical characteristics due to their unique carbon bonding structure. Depending on their chirality and atomic arrangement, CNTs can exhibit either metallic or semiconducting behavior, enabling their application in electronic components, nanoscale transistors, conductive coatings, and sensing systems. Their electrical conductivity can significantly exceed that of traditional conductive materials, providing opportunities for the development of lightweight and efficient electrical networks within composite structures.

CNTs also demonstrate excellent thermal transport capabilities, which have encouraged their use in thermal management applications. Their high thermal conductivity allows efficient heat dissipation, making them suitable for electronic devices and systems where controlling temperature is essential for maintaining performance and reliability. This combination of electrical and thermal properties makes CNTs particularly valuable in multifunctional materials designed to simultaneously provide mechanical reinforcement and enhanced functional characteristics [15].

One of the most promising applications of CNTs is their incorporation into polymer matrices to produce high-performance nanocomposites. Even the addition of relatively small amounts of CNTs can substantially modify the mechanical response of polymer materials by improving stiffness, strength, and resistance to deformation. The high aspect ratio and large interfacial area of CNTs facilitate effective load transfer between the reinforcement phase and polymer matrix, resulting in improved structural performance. Previous investigations have demonstrated that incorporating small CNT concentrations into polymers such as epoxy and polypropylene can lead to significant increases in elastic modulus, tensile strength, and overall durability.

The influence of CNTs extends beyond structural applications, as these nanomaterials have also contributed to advancements in energy-related technologies. Their large specific surface area and superior electrical conductivity make them promising components in energy storage systems, including lithium-ion batteries and supercapacitors, where they can enhance charge transport and storage efficiency. Furthermore, CNT-based materials have been investigated in photovoltaic systems due to their ability to improve electron mobility and charge transfer mechanisms, potentially increasing solar cell performance. Their potential role in hydrogen storage and fuel cell technologies has also been widely explored because of their favorable surface characteristics and interaction with hydrogen molecules [16].

3 | Results and Discussion

3.1 | Mechanical Properties of Nanocomposites

This section is dedicated to evaluating the effective mechanical response of CNT-reinforced polymer nanocomposites and investigating their stability characteristics under buckling conditions. The analysis considers the influence of both material-related parameters and geometric configurations on the structural behavior of the nanocomposite beam. To assess the reliability of the developed micromechanical approach, the predicted elastic properties are compared with available experimental results as well as outcomes obtained from alternative homogenization techniques.

The capability of the Mori–Tanaka (M–T) micromechanical model is further examined through a comparative assessment with the Eshelby-based approach. This verification is performed for epoxy-based nanocomposites containing randomly oriented CNTs. In the considered analysis, the elastic modulus values of CNT reinforcement and the epoxy matrix are assumed to be 1000 GPa and 3 GPa, respectively, while both constituents are assigned a Poisson's ratio of 0.3.

Fig. 2 presents the variation of the normalized effective elastic modulus of the nanocomposite (E/Em) as a function of CNT volume fraction, where E denotes the overall modulus of the reinforced composite and Em corresponds to the modulus of the polymer matrix. The comparison demonstrates a strong agreement between the predictions of the Mori–Tanaka model and the Eshelby formulation, confirming the capability of the proposed micromechanical model in estimating the effective stiffness of CNT-based nanocomposites.

The results further demonstrate that increasing the amount of CNT reinforcement leads to a continuous enhancement in the elastic stiffness of the composite material. This improvement is primarily attributed to the superior mechanical characteristics of CNTs compared with the polymer phase, particularly their extremely high elastic modulus, which enables more efficient load transfer and increases the overall rigidity of the nanocomposite system.

3.2 | Effects of CNT on Mechanical Properties

The influence of key parameters, including temperature variation, CNT volume fraction, nanotube orientation, and interphase characteristics, on the mechanical response of CNT-reinforced nanocomposites was investigated. The results revealed that increasing CNT content improves the elastic modulus due to the superior stiffness of nanotubes compared with the polymer matrix. Moreover, aligned CNTs provide more effective load transfer than randomly distributed nanotubes, resulting in enhanced stiffness and strength. Thermal effects were also found to reduce the mechanical performance of the nanocomposite, mainly due to matrix softening and thermal expansion. In addition, a thicker and stronger interphase region improves stress transfer efficiency, leading to higher composite stiffness and strength.

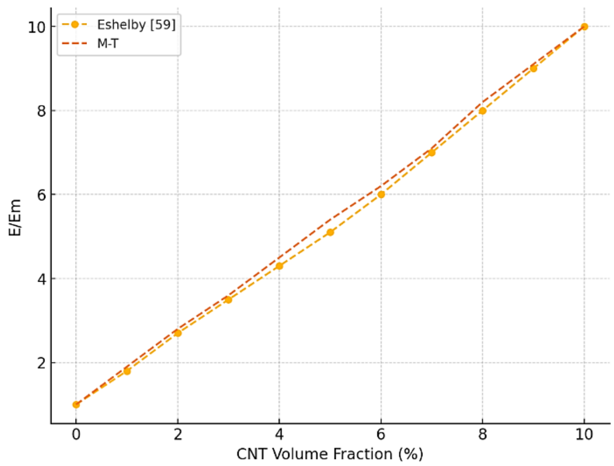

Fig. 2. Comparison of micromechanical model results for the effective elastic response of CNT-reinforced nanocomposites.

Table 1. Mechanical properties of CNT and epoxy resin.

Material	Longitudinal Elastic Modulus (E_L) (GPa)	Transverse Elastic Modulus (E_T) (GPa)	Longitudinal Poisson's Ratio (v_L)	Transverse Poisson's Ratio (v_T)
CNT	240	50	0.162	0.47
Epoxy Resin	2.5	2.5	0.34	0.34

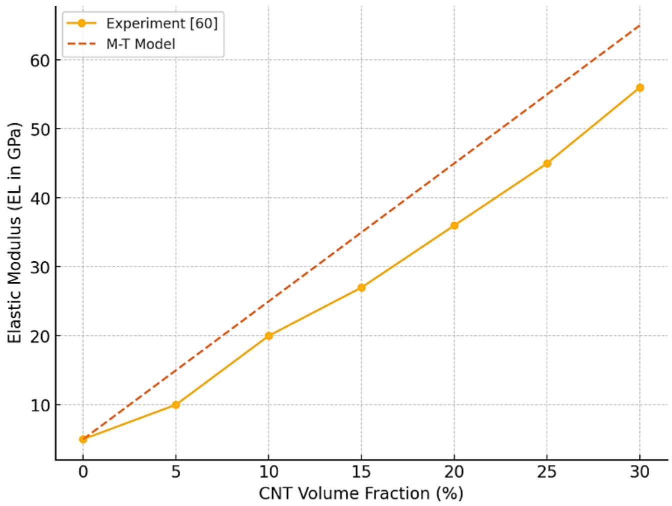

Fig. 3. Comparison of measured and predicted elastic responses of CNT/epoxy nanocomposites using the Mori–Tanaka homogenization scheme.

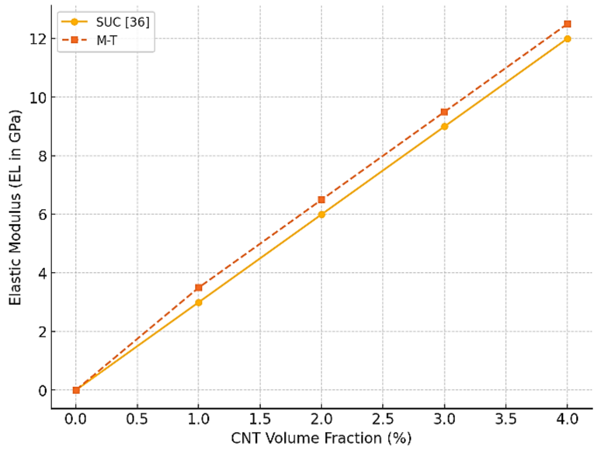

Fig. 4. Comparative assessment of micromechanical model predictions for the elastic response of CNT-reinforced nanocomposites.

Table 2. Longitudinal and transverse elastic properties of CNTs and epoxy matrix.

Material	EL(GPa)	ET(GPa)	vL	vT
CNT	800	49	0.16	0.45
Epoxy Resin	2.5	2.5	0.34	0.34

Further validation of the proposed Mori–Tanaka (M–T) micromechanical model was performed by comparing its predictions with the Simplified Unit Cell (SUC) approach for the longitudinal elastic modulus of aligned CNT-reinforced Shape Memory Polymer (SMP) nanocomposites. The polymer matrix was considered isotropic, with an elastic modulus of 0.622 GPa and a Poisson's ratio of 0.3. As illustrated in *Fig. 4*, both models exhibit consistent predictions, confirming the reliability of the M–T formulation. The results also indicate that increasing CNT content leads to a continuous improvement in the effective elastic modulus of the nanocomposite.

In addition, the capability of the proposed model was assessed using experimental data reported for CNT/polypropylene nanocomposites. The polypropylene matrix properties were defined as an elastic modulus of 1.85 GPa and a Poisson's ratio of 0.45, while CNTs were modeled as transversely isotropic reinforcements with an average diameter of 50 nm. The effects of interfacial characteristics were considered through an adhesion parameter of 23.28 and an interphase thickness of 2.38 nm. The predicted elastic modulus obtained from the M–T model showed good agreement with experimental observations, as presented in *Fig. 5*. Furthermore, the results confirmed that CNT incorporation enhances the stiffness of the polymer matrix due to the superior mechanical properties of the nanotubes.

The longitudinal and transverse elastic moduli, along with the corresponding Poisson's ratios of CNTs and epoxy resin, are summarized in *Table 2*. Overall, the comparisons presented in *Figs. 2–5* demonstrate that the proposed micromechanical model provides reliable predictions and can be effectively employed for estimating the effective properties of CNT-reinforced nanocomposites.

4 | Conclusion

This study investigated the buckling response of CNT-reinforced polymer nanocomposite beams using the Mori–Tanaka micromechanical model combined with finite element analysis. The results demonstrated that CNT incorporation significantly improves the stiffness and critical buckling load of nanocomposite beams due to the superior mechanical characteristics and efficient load transfer capability of nanotubes.

The presence of an interphase layer between CNTs and the polymer matrix was found to be a key factor in enhancing structural performance by improving stress transfer and increasing buckling resistance. Conversely, elevated temperatures reduced the buckling capacity due to the thermal softening of the polymer matrix. Parametric analyses also revealed that smaller CNT diameters, thicker interphase regions, larger beam cross-sections, and shorter beam lengths contribute to improved stability performance. Moreover, hollow square sections exhibited better behavior than solid sections in higher buckling modes.

The mesh convergence study confirmed that increasing the number of finite elements beyond approximately 5000 elements provides negligible improvement in prediction accuracy, allowing an effective balance between computational cost and reliability. Overall, the findings highlight the importance of CNT content, interfacial characteristics, thermal conditions, and structural geometry in optimizing the buckling performance of CNT-reinforced nanocomposite structures for advanced engineering applications.

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