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RESEARCH PAPER

Machine Learning Insights into the Influence of Carbon Nanotube Dimensions on Nanocomposite Properties: A Comprehensive Exploration

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Abstract

Multiscale modeling (MM) has broadened its scope to encompass the calculation of mechanical properties, with a particular focus on investigating how the dimensions of single-walled carbon nanotubes (SWCNTs), specifically their diameters, affect the mechanical properties (Longitudinal and Transverse Young's modulus) of simulated nanocomposites through Molecular Dynamics (MD) simulations. The MD method was employed to construct nanocomposite models comprising five different SWCNTs chiralities: (5, 0), (10, 0), (15, 0), (20, 0), and (25, 0), serving as reinforcements within a common Polymethyl methacrylate (PMMA) matrix. The findings indicate a correlation between the SWCNT diameter increase and enhancements in mechanical and physical properties. Notably, as the diameter of SWCNTs increases, the density, Longitudinal Young's modulus, Transvers Young's Shear modulus, Poisson's ratio, and Bulk modulus of the simulated nanocomposite transition from (5, 0) to (25, 0) by approximately 1.54, 3, 2, 1.43, 1.11, and 1.75 times, respectively. To corroborate these results, stiffness matrices were derived using Materials Studio software.

Keywords: Molecular dynamics simulation, Mechanical properties, Polymethyl methacrylate, single walled carbon nanotubes

1. Introduction

Molecular dynamics simulation is a powerful computational technique used to study the behavior of atoms and molecules over time. It employs Newton's laws of motion to track the positions and velocities of particles in a system, allowing researchers to simulate the dynamic evolution of molecular systems under various conditions. By numerically solving the equations of motion for a system of interacting particles, molecular dynamics simulations provide insights into the structural, thermodynamic, and kinetic properties of materials at the atomic scale [1-3]. Recently, nanostructured materials, particularly carbon nanotube (CNT)-reinforced nanocomposites, have garnered attention as a novel generation of materials among researchers [4, 5]. CNTs possess exceptional properties including

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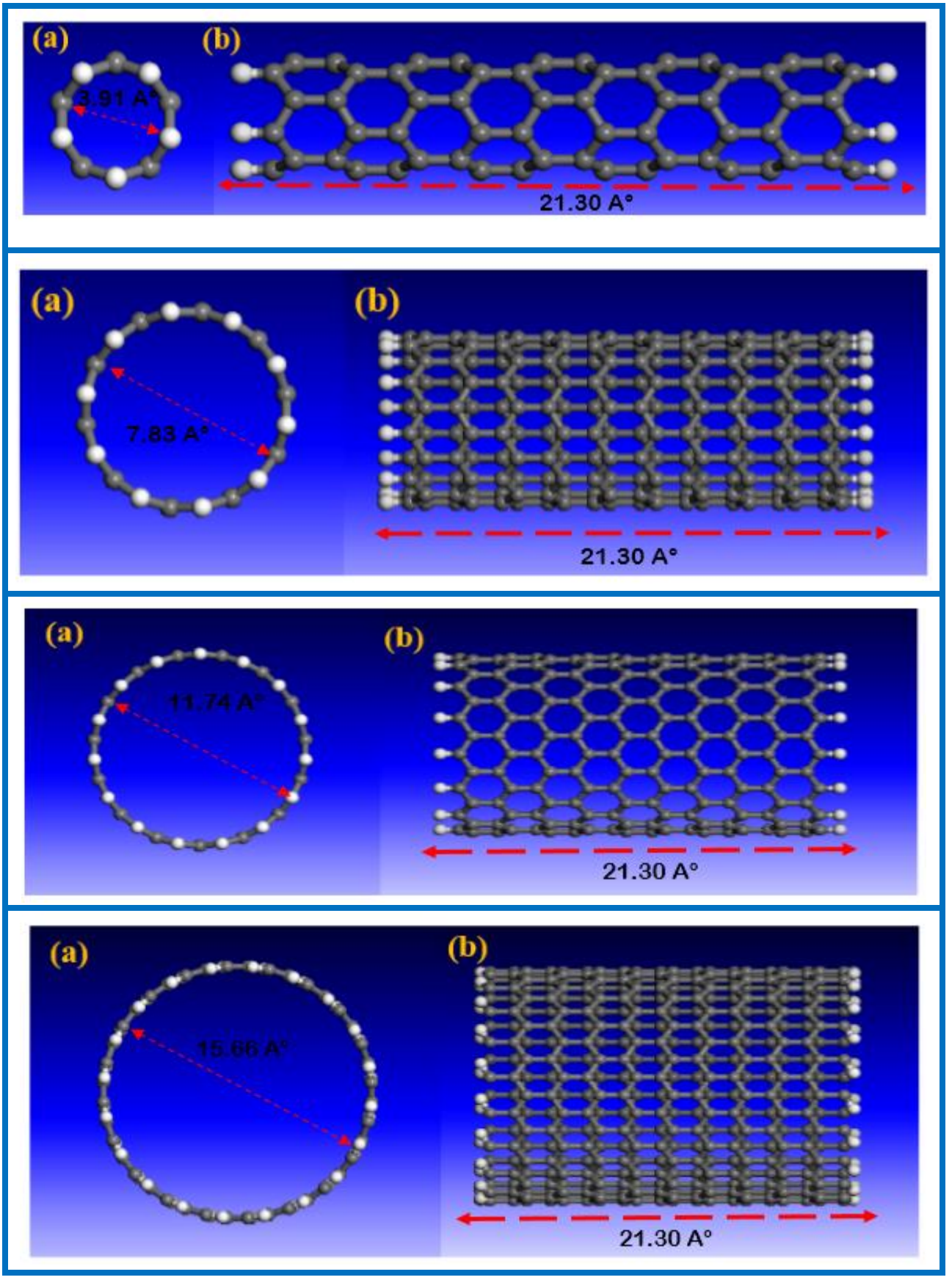
high stiffness, strength, and thermal and electrical conductivity, rendering them ideal candidates for polymer-based nanocomposites [6]. The mechanical properties of such nanocomposites are affected by various parameters such as the size, distribution, orientation, and morphology of the reinforcement [7-10]. In CNT-reinforced composites, factors like chirality and aspect ratio significantly influence elastic properties such as Young's modulus [11]. Atomistic and multiscale modeling (MM), particularly employing molecular dynamics (MD) simulations, have been instrumental in predicting the physical and mechanical properties of thermoset polymeric structures [12-16]. Several studies have utilized MD to model nanocomposite samples at the nanoscale [17-19]. For instance, Mahboob and Islam investigated the mechanical properties of CNT-reinforced polyethylene (PE) composites using MD, revealing a decrease in Young's modulus with increasing defects in the CNTs [20]. Arash et al. [21] explored the mechanical properties of CNT/poly (methyl methacrylate) (PMMA) composites via MD, analyzing the effects of CNT aspect ratio on Young's modulus using the Mori–Tanaka (MT) method. Al-Haik et al. [22] examined how CNT construction influences radiation-induced damage in composites based on PE and single-walled carbon nanotubes (SWCNTs) with different chiralities using MD. Despite the exceptional mechanical properties attributed to CNTs, experimental results have shown only modest improvements in the effective elastic moduli of nanocomposites, which could be attributed to CNT agglomeration. Shi et al. [23] proposed an analytical method to study the effects of CNT agglomeration on nanocomposite elastic properties using the MT method, suggesting that increased agglomeration could lead to a significant decrease in Young's modulus. While MD is a potent method for nanoscale material modeling and simulation, it is limited by its applicability to small sizes [24-27]. To address this limitation, multiscale methods have been developed. Typically, multiscale modeling involves two main steps: atomistic simulation at the nanoscale and continuum methods such as micromechanics or finite element methods (FEM) at the micro or macroscale. Odegard et al. [28] introduced the effective fiber method for modeling polymer-based nanocomposites reinforced with CNTs, combining molecular computations with continuum methods to examine elastic behavior across different scales.

This paper presents a comprehensive study of how carbon nanotube dimensions affect the mechanical properties of nanocomposites using the MD method. Simulated nanocomposite models comprising five SWCNT case studies with different chiralities [(5, 0), (10, 0), (15, 0), (20, 0), and (25, 0)] as reinforcement, along with Polymethyl methacrylate (PMMA) as the matrix, were created using MD. The total weight of the nanocomposite is assumed to be 8 grams, with 2 grams allocated to SWCNTs as reinforcement.

2. Materials and Methods

2.1. Software, Force Field, and Simulation steps

In this article Materials Studio 6.0 has been used for carrying out the molecular (MDs) simulation. To study mechanical properties (Longitudinal and Transverse Young's modulus) of armchair SWCNTs with different chiralities (5, 0), (10, 0), (15, 0), (20, 0) and (25, 0) with diameter of 3.91, 7.83, 11.74, 15.66 and, 19.57 A° and the same length of 21.30 A° for each five case study as shown in Fig. 1 have been used respectively. To avoid the influences of unsaturated boundary conditions, both the ends of CNT were terminated by hydrogen atoms. It is the most common force field, has been applied for defining the inter and intra-molecular atomic interactions. The ensemble of NVE reveals that the sum of kinetic (KE) and potential energies (PE) is conserved, T and P are unregulated, and N, V, and E denote a constant number, volume, and energy, respectively. At this step, the simulation box is placed at a temperature of 300 K under NVE. The simulation time is considered 100 ps. NVT represents that temperature (T) is regulated via a thermostat, which typically adds a degree of freedom to the conserved Hamiltonian; KE and PE are included in the Hamiltonian; P is unregulated. At this part, the simulation box is set at a temperature of 300 K under NVT. The initial density of the system (0.9gr / cm^3) is assumed to allow molecules and atoms to be displaced to move towards optimal mode. The simulation time considered 100 ps. NPT is like NVT, but the pressure (P) is regulated. Density is one of the physical properties that is considered in atomic modeling. It defines the accuracy of the density of the atoms in equilibrium. If the atomic modeling path is followed correctly, the density of the atomic system is expected to be close to the actual density of the system in comparison to the macro. Furthermore, it is assumed that after the simulation time the amount of any quantity attributed to the system of atoms, including the converged density of the solution fluctuations, will decrease over time. At this point, the system is pressurized at atmospheric pressure 1 at a temperature of 300 K under a constant NPT to close the system density to the actual density. NPT can also eliminate system tensions. The simulation time at this stage is considered 100 ps.


(a)
(b)
3.91 A°
21.30 A°
(a)
(b)
7.83 A°
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11.74 A°
21.30 A°
(a)
(b)
15.66 A°
21.30 A°

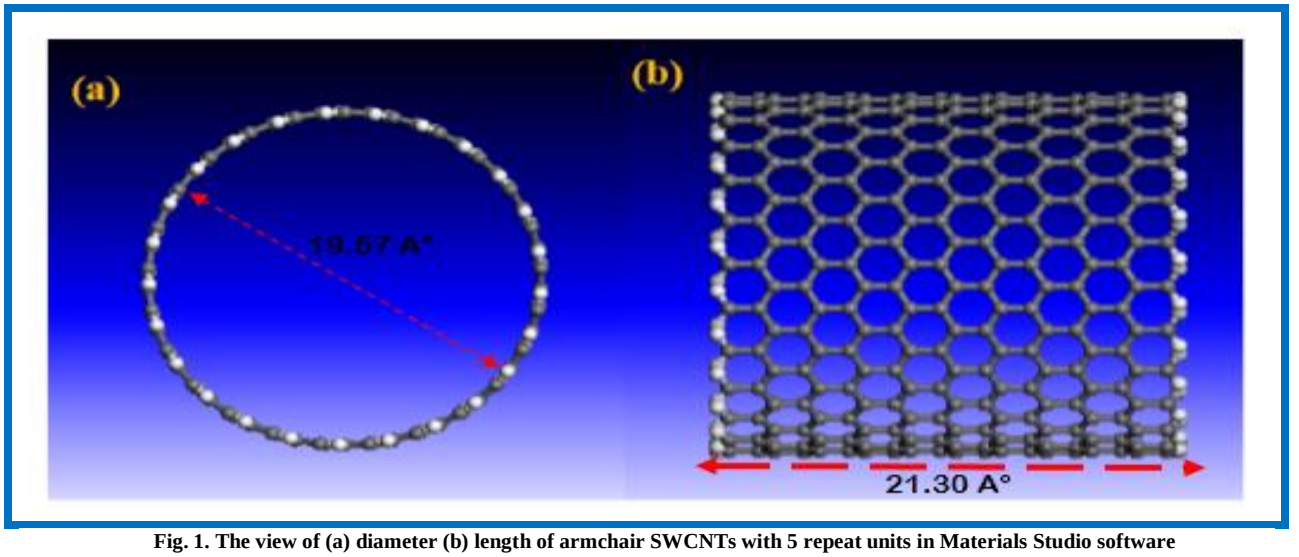


Fig. 1. The view of (a) diameter (b) length of armchair SWCNTs with 5 repeat units in Materials Studio software

A single chain of the polymer, consisting of 50 chain length of Polymethyl methacrylate (PMMA), a widely used synthetic thermoplastic polymer has been used as a matrix as shown in Fig. 2. Condensed Phase Optimized Molecular Potential for Atomistic Simulation Studies (COMPASS). PMMA as the matrix material in this study likely stems from its desirable combination of mechanical properties, thermal stability, processability, transparency, chemical resistance, and biocompatibility, making it a versatile and relevant choice for investigating the influence of carbon nanotube dimensions on nanocomposite properties.

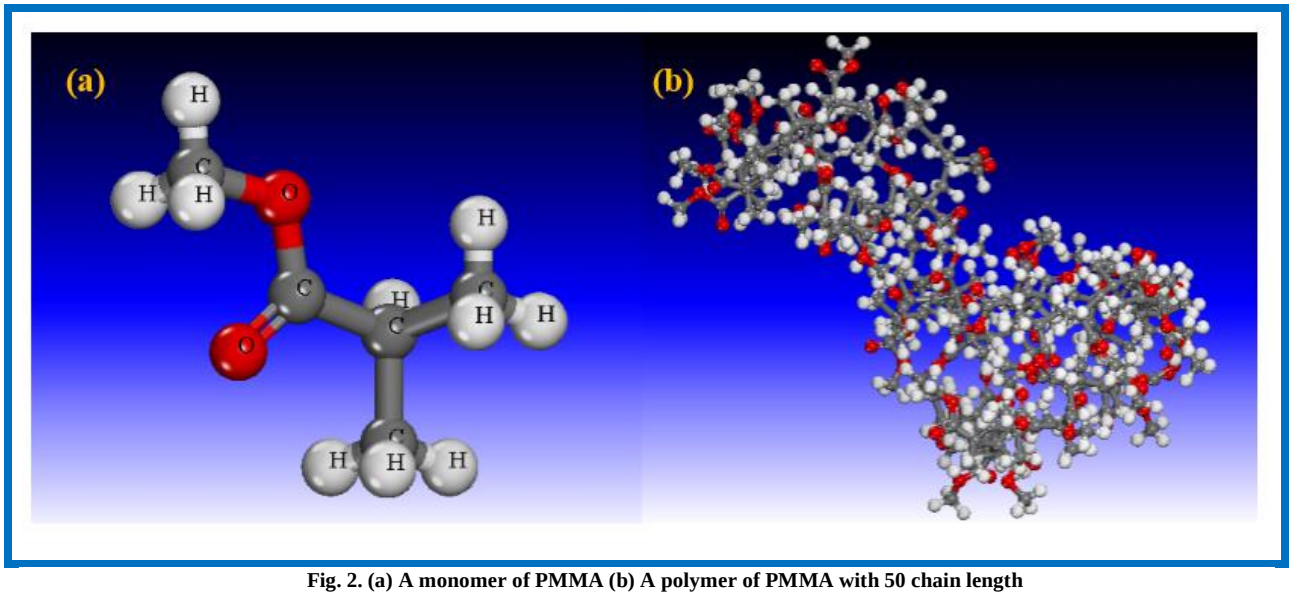


Fig. 2. (a) A monomer of PMMA (b) A polymer of PMMA with 50 chain length

The following steps have been taken to complete the MDs method for obtaining mechanical and physical properties as shown in Fig. 3.

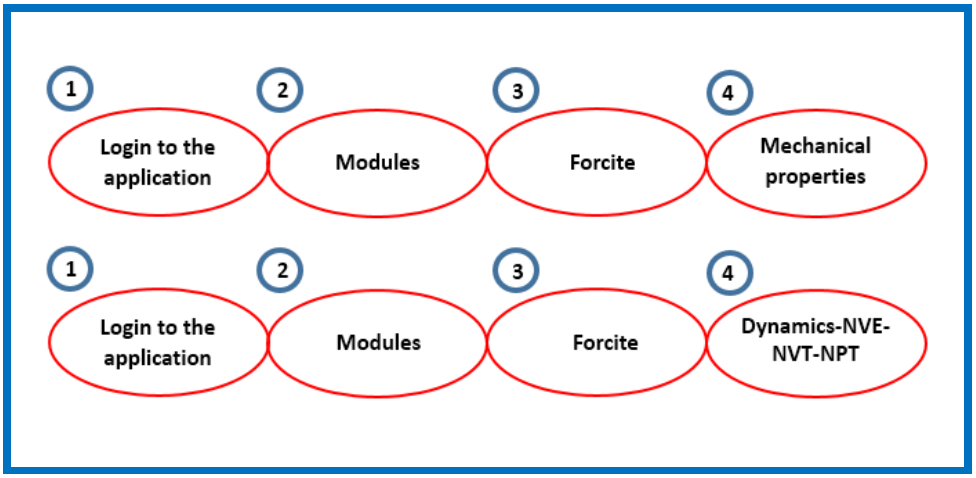
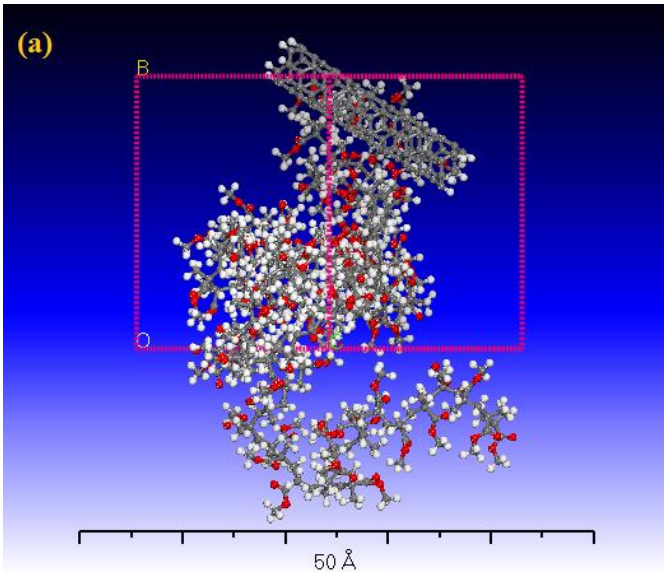
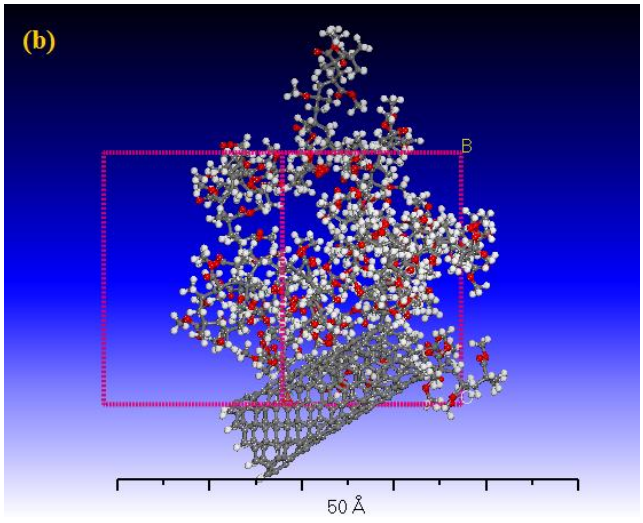


Fig. 3. Four steps to reach mechanical and physical properties using Materials Studio software

2.2. Simulation methodology

In this part, the effect of the diameter of CNTs on their mechanical properties (Longitudinal and Transverse Young's modulus) is investigated by the MDs method as shown in Fig. 4. To simulate nanocomposite in MDs software, and for accurate calculations the total weight percent of reinforcements was 25% of the total weight and constant amount (75%) for the polymer. It should be noted that the overall weight of the simulated composites is 8 gr, and the weight of the polymer (PMMA) is 6 gr.




(b)
B
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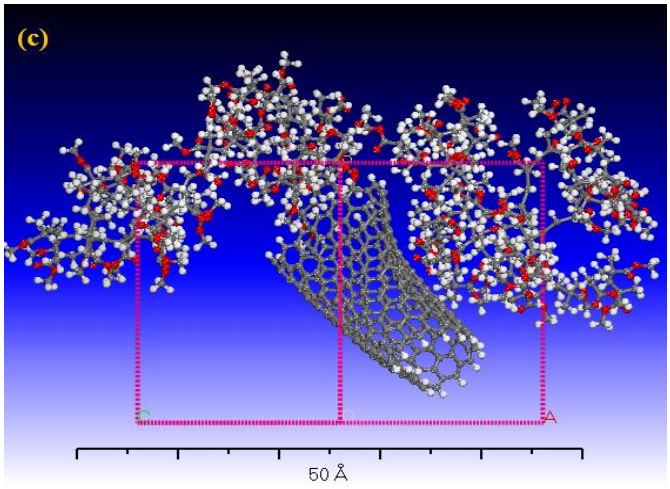
(c)
A
50 Å

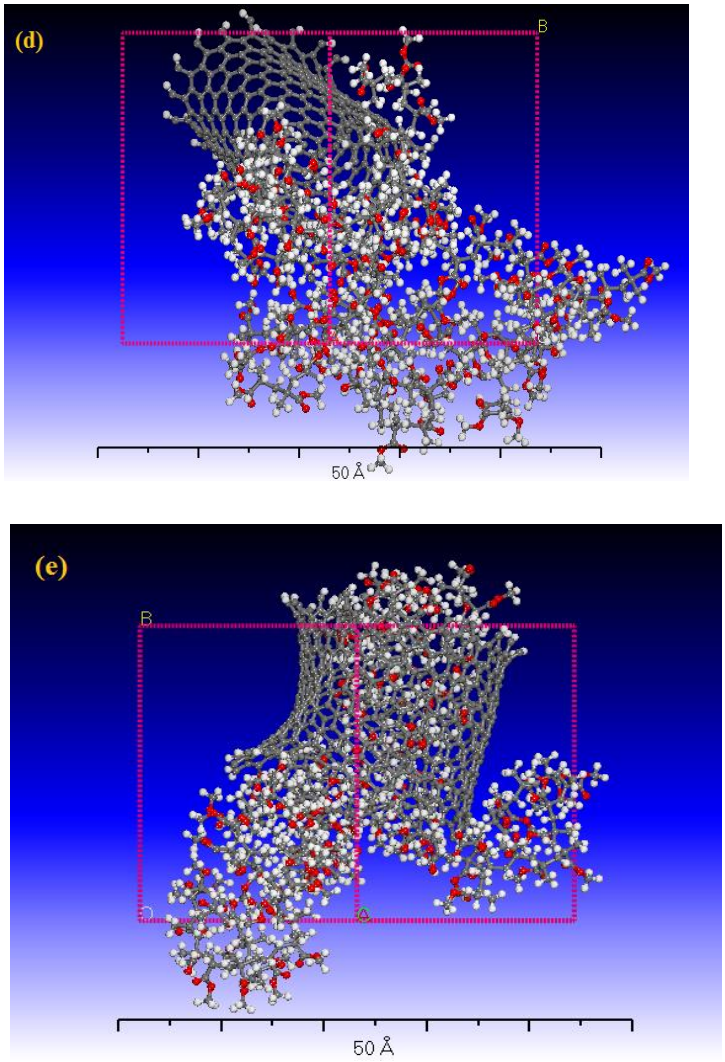

Fig. 4. Five simulated boxes with different chiralities (a) (5, 0), (b) (10, 0), (c) (15, 0), (d) (20, 0) and (e) (25, 0) using Materials Studio software

3. Result and Discussion

The mechanical properties (Longitudinal and Transverse Young's modulus) of SWCNTs with different chiralities (5, 0), (10, 0), (15, 0), (20, 0) and (25, 0) as the reinforcement and using Polymethyl methacrylate (PMMA) as the common matrix are investigated as shown in Fig. 5. The longitudinal Young's modulus is calculated 3.7, 5.1, 6.3, 7.9 and 9.5 GPa respectively which shows a threefold increase. The transverse Young's modulus is calculated 3.3, 3.8, 4.1, 5.9 and 9.1 GPa respectively which shows approximately twofold increase.

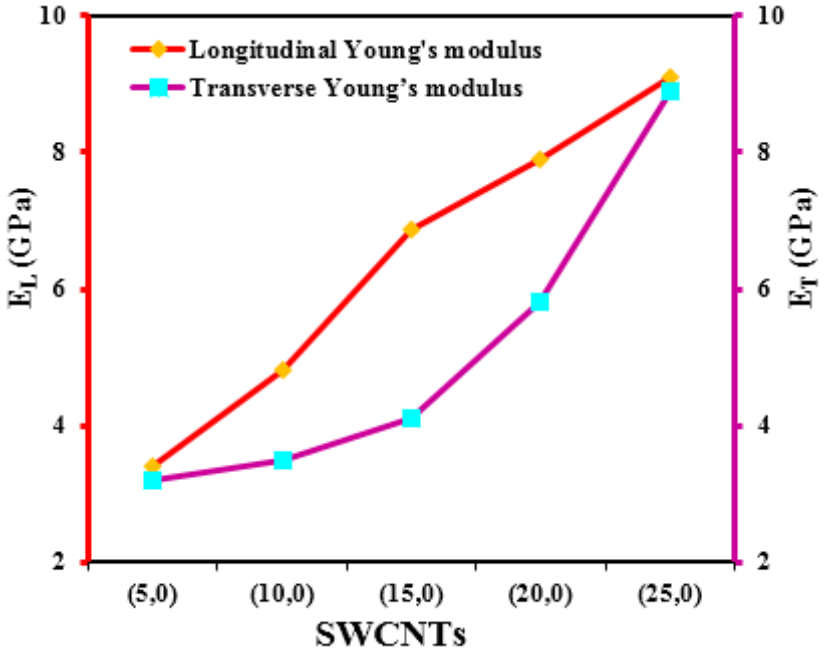

Fig. 5. Result of Longitudinal and Transvers Young's modulus (SWCNTs- PMMA)

In this part the extra calculations were done and to reduce the number of graphs, the sample with chirality (25, 0) was chosen and the obtained results were discussed for further investigations. To draw the density diagram, first, the simulated NVT to maximize the energy of system and then the NPT was plotted to show the density. As shown in Fig. 6 the density was predicted approximately 1.25 g/cm^3.

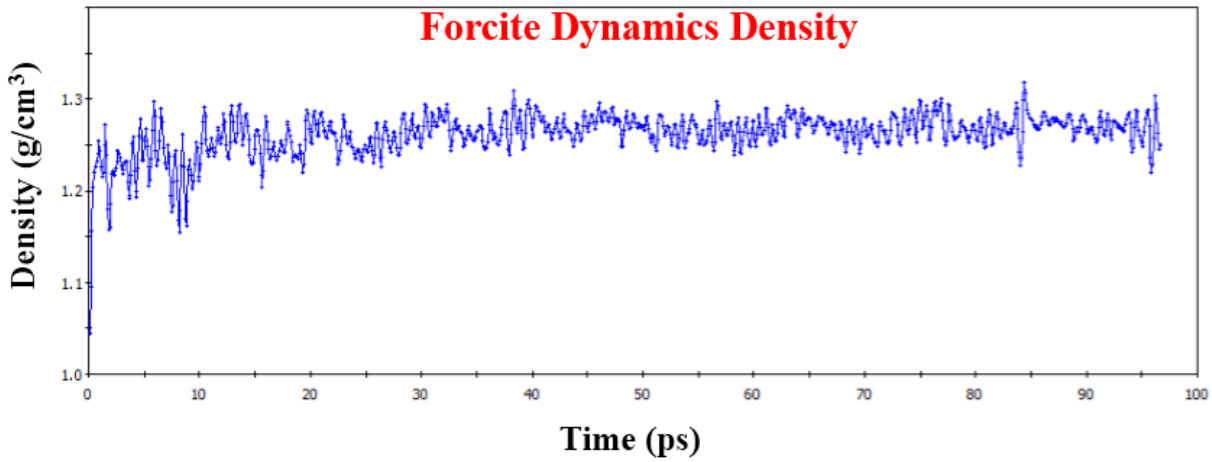

Fig. 6. Density diagram armchair SWCNTs (25, 0) mixed with PMMA

To validate the simulation results, elastic stiffness matrix was determined using a constant strain method. The elastic stiffness matrix components were defined for SWCNTs (25, 0) with PMMA as a polymer matrix, under a strain of 60.003 and at a pressure of 1 atm. These results are as follows:

$$C_{ij}(GPa) = \begin{bmatrix} -6.2811 & 0.5504 & 3.8897 & 1.1397 & -0.6569 & -0.6992 \\ 0.5504 & -8.8962 & -6.6375 & -4.2861 & 0.7676 & 0.4550 \\ 3.8897 & -6.6375 & -6.6422 & -1.3783 & 1.6240 & -0.3777 \\ 1.1397 & -4.2861 & -1.3783 & 1.5629 & 3.3594 & 3.0916 \\ -0.6569 & 0.7676 & 1.6240 & 3.3594 & 1.2339 & -2.1884 \\ -0.6992 & 0.4550 & -0.3777 & 3.0916 & -2.1884 & 1.6108 \end{bmatrix}$$

As can be seen, because of the isotropy of the material, the diagonal elements are nearly similar, and the matrix is approximately symmetric. Finally, the other significant mechanical and physical properties are calculated and due to reduce diagrams all information gather in Table 1 and shows with increasing diameter of CNTs all mechanical and physical properties increased.

Table 1: Details of significant mechanical and physical properties of five case study for simulated nanocomposites

Type of CNT	Density (g/cm^3)	Poisson's ratio	Shear modulus (GPa)	Bulk modulus (GPa)
(5,0)	0.81	0.27	4.20	2.90
(10,0)	0.83	0.28	4.29	3.30
(15,0)	0.97	0.28	5.05	3.78
(20,0)	1.04	0.28	5.09	4.26
(25,0)	1.25	0.30	6.03	5.08

Conclusion

In this research, the molecular dynamics (MDs) simulation for predicting the effect of diameter of armchair SWCNTs with different chiralities (5, 0), (10, 0), (15, 0), (20, 0) and (25, 0) on the mechanical and physical properties of SWCNTs as reinforcements with common polymer (PMMA) were simulated based on materials studio software. With these good looking and easily understandable atom models, the mechanical and physical properties of simulated nanocomposites were calculated and compared individually. The most important results are as follows:

1-Predicting the effect of diameter of SWCNTs on mechanical and physical properties of five cases was simulated by materials studio software.

2- Physical properties improve with increasing diameter of SWCNTs

3- Mechanical properties increase due to high Young's modulus of SWCNTs

4- With the increasing diameter of SWCNTs, Longitudinal Young's modulus from (5, 0) to (25, 0) becomes approximately 3 times more than (5, 0).

5- With the increasing of diameter of SWCNTs, Transverse Young's modulus from (5, 0) to (25, 0) becomes approximately 2 times more than (5, 0).

6- With the increasing of diameter of SWCNTs, Shear modulus from (5, 0) to (25, 0) becomes 1.43 times more than (5, 0).

7- With the increasing diameter of SWCNTs, Poisson's ratio from (5, 0) to (25, 0) becomes 1.1 times more than (5, 0).

8- To validate the results, the stiffness matrix is obtained by MD simulation for (25, 0) simulated nanocomposite calculated and observed, because of the isotropy of the material, the diagonal elements are nearly similar, and the matrix is approximately symmetric.

Future research endeavors could delve deeper into the integration of advanced machine learning methodologies with molecular dynamics simulations to enhance predictive capabilities and uncover subtle nuances in nanocomposite behavior. Additionally, exploring the effects of environmental factors, such as temperature and humidity, on the properties of nanocomposites could provide valuable insights into their real-world applicability. Furthermore, extending our analysis to include a broader range of nanotube configurations and composite matrices could offer a more comprehensive understanding of the design space and facilitate the development of tailored materials with enhanced functionalities. In summary, the integration of machine learning techniques with molecular dynamics simulations opens up exciting possibilities for advancing our knowledge of nanocomposite systems. By continuing to explore these interdisciplinary approaches, we aim to address current challenges and pave the way for the design and optimization of next-generation materials with tailored properties for various applications.

Conflict of Interest

The authors declared no potential conflicts of interest with respect to the research, authorship, and publication of this article.

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