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Nano research for investigating the effect of SWCNTs dimensions on the properties of the simulated nanocomposites: a molecular dynamics simulation

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Abstract. This research investigates the effect of single walled carbon nanotubes (SWCNTs) dimensions in terms of diameter on the mechanical properties (longitudinal and transverse Young's modulus) of the simulated nanocomposites by molecular dynamics (MDs) method. MDs utilized to create nanocomposite models consisting of five case studies 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. The results show that with increasing of SWCNTs diameter, the mechanical and physical properties increase. It is important that with the increasing of SWCNTs diameter, density, longitudinal and transverse Young's modulus, shear modulus, poisson's ratio, and bulk modulus of simulated nanocomposite from (5, 0) to (25, 0) approximately becomes 1.54, 3, 2, 1.43, 1.11 and 1.75 times more than (5, 0), respectively. Then to validate the results, the stiffness matrix is obtained by Materials studio software.

Keywords: molecular dynamics simulation; mechanical properties; polymethyl methacrylate; single walled carbon nanotubes; different chiralities

1. Introduction

Lately, nanostructured and nanoscale materials such as carbon nanotubes (CNTs) have been considered as a novel generation of materials by researchers (Aghadavoudi *et al.* 2018, Emdadi *et al.* 2019, Marani and Perri 2017). CNTs have remarkable properties such as great stiffness, high strength, excellent thermal and electrical properties (Tayeb *et al.* 2020). Consequently, these properties make CNTs great applicants and the best reinforcement for nanocomposites (Mohammadimehr *et al.* 2020, Rostami and Mohammadimehr 2020, Shahedi and Mohammadimehr 2019). Mechanical and physical properties of nanocomposites are influenced by various parameters such as reinforcement size, arrangement, orientation, and morphology (Farazin *et al.* 2020). In CNTs chirality and aspect ratio have a high effect on elastic properties such as Young's modulus (Aghadavoudi *et al.* 2019). Atomistic and multiscale modeling (MM) especially molecular dynamics (MDs) method has been applied to obtain the significant properties of nanostructures before fabrication by numerous scholars and also some investigators utilized MDs for modeling the nanocomposite samples at the nanoscale (Sutrakar *et al.* 2015). Mahboob and Islam (2013) defined properties of CNT-reinforced polyethylene (PE) composite utilizing MDs. Their outcomes revealed an increase in the number of defects in the CNTs leads to a reduction in mechanical properties of nanocomposites. Arash *et al.* (2014) applied MDs to examine the mechanical properties of CNT/PMMA composite. They investigated the elastic constants for the CNT/matrix interfacial area and investigated the influences of the CNT aspect ratio on the mechanical properties of nanocomposite applying the Mori–Tanaka (MT) method. Al-Haik *et al.* (2015) examined the influences of CNTs construction on the radiation-induced damage of composites based on PE and SWCNTs with different chiralities employing MDs. Although outstanding mechanical and physical properties have been described utilizing CNTs, experimental tests reveal a reasonable improvement in Young's modulus of nanocomposites (Ghorbanpour Arani *et al.* 2019). This weak enhancement in nanocomposite properties could be due to CNT agglomeration. In the other work, Ghorbanpour Arani *et al.* (2016) considered surface stress and agglomeration effects on nonlocal biaxial buckling polymeric nanocomposite plate reinforced by CNT using various approaches. Shi *et al.* (2004) revealed an analytic method for investigating the influences of CNT agglomeration on the mechanical properties of nanocomposites based on the MT method. They explained that growing agglomeration may result in a considerable decrease in nanocomposite Young's modulus. AkhavanAlavi *et al.* (2019) presented active control of micro Reddy beam integrated with functionally graded nanocomposite sensor and actuator based on linear quadratic regulator method.

MD is a strong method for modeling and simulation nanostructures in nanoscale, however, molecular simulation is limited to small size, in microscale, multiscale methods have been expanded to solve this restriction (Farzinpour *et al.* 2020). Commonly, multiscale modeling consists of two principal steps (Mehar and Panda 2019). Atomistic

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simulation takes into account the discrete nature of nanocomposite molecular structures at the nanometer length scale (Hadipeykani *et al.* 2020, Low and Shon 2018). At the micro or macro step, continuum methods such as finite element methods (FEM) or micromechanics can be applied to estimate the mechanical and physical properties of simulated nanocomposites. Odegard *et al.* (2017) introduced the effective fiber method for simulation nanocomposites with CNTs as reinforcement. They applied molecular calculations for generating an effective reinforcement model and they estimated five elastic constants for this molecular model. In the next step, they applied the MT method to examine the mechanical behavior of nanocomposite at micro- and macroscales. Their research was the first attempt to examine the mechanical properties of nanocomposites applying multiscale modeling. Mohammadimehr *et al.* (2018a, b) studied bending, buckling, and free vibration analyses of carbon nanotube reinforced composite beams and experimental tensile test to obtain the mechanical properties of nanocomposite. Babaeeian and Mohammadimehr (2020) investigated the time elapsed effect on residual stress measurement in a composite plate by DIC method. Farazin *et al.* (2019) investigated the mechanical behavior of porous bio-nanocomposite by MDs to compare with the results of the experimental analysis. Their results indicated some theories like Dewey's method are incorrect for the mechanical properties for porous nanocomposite. Yu *et al.* (2009) studied the size of nanoparticle on the mechanical and physical properties of thermoset epoxy-based nanocomposite employing MDs. Mohammadimehr and Alimirzaei (2016) illustrated nonlinear static and vibration analysis of Euler-Bernoulli composite beam model reinforced by FG-SWCNT with initial geometrical imperfection using finite element method. Yang *et al.* (2012) revealed a multiscale model to examine the size of CNTs on the stiffness of nanocomposites. They applied an effective fiber method for multiscale modeling and determined that Young's moduli of CNT and adsorption layer near CNT contributed to the elastic behavior of nanocomposites. Aghadavoudi *et al.* (2016) tested the effect of defected carbon nanotubes (CNT) on the mechanical properties of nanocomposites with thermoset matrix by MD and evaluating the elastic modulus changes, as an example investigation of shear modulus in the use of defected CNTs. Montazeri *et al.* (2011) evaluated the effect of CNTs orientation on the shear deformation properties of thermoplastic polymers by the combination of MD and finite element analysis (FEA). Their result illustrated that in the 45° direction, single-wall carbon nanotubes (SWCNT) had the greatest impact on the shear modulus. Mortazavi *et al.* (2015) investigated MDs for thermal conductivity and mechanical features of CNT with thermoset polymers and investigated the proper mechanical performance. Rajabi and Mohammadimehr (2019) presented bending analysis of a micro sandwich skew plate using extended Kantorovich method based on Eshelby-Mori-Tanaka approach. Khandan *et al.* (2020) fabricated and simulated mitral heart value with thermoplastic polyurethane by 3D bio printer. Their results help heart patients significantly. Frankland *et al.* (2003) studied the stress and strain behaviors of thermoset polyethylene-based nanotube composite strain by adding single-walled and multi-walled carbon nanotubes (SWCNT/MWCNT) using MDs and increasing the hardness of polymer in longitudinal lengths of carbon nanotubes. Marcadon *et al.* (2013) applied an MD approach to investigate the effect of nanoscale particles on the properties of thermoset polymer nanoparticles. In their research, silica nanoparticles in polymer and simulation of MD are applied. Their results showed that particle size effect on the mechanical behavior of nanocomposites; which shows the proper effect of Young's modulus increases with particle size. Haghighi *et al.* (2020) investigated the effects of defects and functional groups on graphene and nanotube thermoset epoxy-based nanocomposites mechanical properties using molecular dynamics simulation. The results of their research showed that defects and functional groups reduce the elastic modulus of the nanofillers and nanocomposites in continuous nanofiller-reinforced epoxy. Iuvshin *et al.* (2020) examined comparative analysis between thermoplastics and thermosets polymer materials. They examined the problems of the choice of the polymer matrix (thermoset and thermoplastic) and reinforcement filler in the manufacture products were made of polymer composite materials for the oil industry. Honma *et al.* (2020) investigated the effects of thermoplastic resin properties on fracture mode and welding strength with welding technology of thermoset fiber-reinforced plastic. Their results suggested that a suitable thermoplastic resin can increase welding strength in the welding technology of thermoset fiber-reinforced plastic. Schichtel and Chattopadhyay (2020) investigated the modeling thermoset polymers using an improved molecular dynamics crosslinking methodology. They analyzed glass transition temperatures and mechanical properties of some thermoset polymers. Nawafleh and Celik (2020) examined additive manufacturing of short fiber reinforced thermoset composites with unprecedented mechanical performance and they showed that the mechanical properties of the additively fabricated thermoset composites match those of ubiquitous, denser structural metals, and these properties show nearly isotropic behavior. Chan *et al.* (2020) reviewed mechanical properties of wollastonite reinforced thermoplastic composites. They concluded that the properties of wollastonite-filled polymer composites were the function of filler content, adhesion interactions of wollastonite particles with polymer matrix, size and shape of wollastonite particles.

A review of studies on the literature review shows that most previous research has focused on mechanical properties of resin epoxy which reinforced by CNTs. This paper provides a comprehensive study of the effect of SWCNTs dimensions on the mechanical and physical properties of nanocomposites by the MDs method. Therefore, MDs method is utilized to create simulated nanocomposite boxes consisting of five case studies 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.

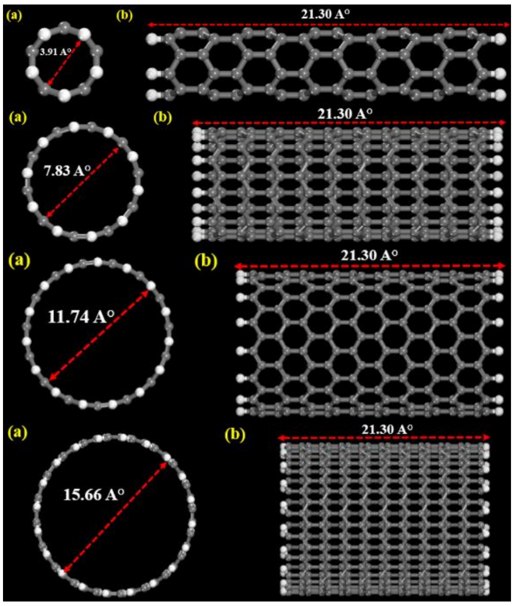

Fig. 1 The view of (a) various diameter (b) constant length of armchair SWCNTs in materials studio software

It should be noted that the overall weight of the nanocomposite is assumed to be 8 gr. Total weight of SWCNTs are 2 gr and selected as reinforcement. The use of SWCNTs and their properties are known in many medical studies such as biosensors and drug release (Smart *et al.* 2006, Firme and Bandaru 2010).

2. Materials and methods

2.1 Software, force field and simulation steps

In this article, Materials Studio 6.0 has been used for calculation 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° have been used for each five case study as shown in Fig. 1, respectively. To avoid the influences of unsaturated boundary conditions, both the ends of SWCNTs 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 (0.9 gr/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 similar to 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 considered 100 ps.

For obtaining the best results, the best force field to exact predict physical and mechanical properties had to choose, one of the best and most accurate force fields, is Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies (COMPASS) force field. On the other hands, the initial atomistic models are simulated in Materials Studio software and COMPASS force field is determined for modeling intermolecular atomic interactions. The best reason for choosing COMPASS because this force field is very suitable for ceramic and polymer matrix. The COMPASS parameters for covalent molecules are completely confirmed using various calculation techniques including extended molecular dynamics simulations of liquids, crystals, and polymers. COMPASS is the first ab-initio force field able to foretelling thermo-mechanical properties of polymers like polymer nanocomposites perfectly. The COMPASS force field has extensive coverage in covalent molecules including most common organic and small inorganic molecules. Moreover, COMPASS force field is capable of being used in the consolidated coverage of organic and inorganic materials models. For these molecular systems, the COMPASS force field has been parameterized to predict different properties for molecules in condensed phases. The values of these parameters are included in the molecular dynamics software databases such as Materials Studio. Intermittently, the parameter set of COMPASS force field for calculating the atomistic forces is revised using updating or addition of new functional groups; consequently, various versions of COMPASS are retained and made available for the purposes of validations and investigation. The used energy potential function E_{total} in COMPASS, includes the valence energy, cross-coupling energy and non-bonded energy as follows by Hadipeykani *et al.* (2020).

$$E_{total} = E_{valence} + E_{cross} + E_{non-bond} \tag{1}$$

$$E_{valence} = E_{bond} + E_{angle} + E_{torsion} + E_{out-of-plane} \tag{2}$$

The terms of energy in Eqs. (1) and (2) are

$$E_{bond} = \sum_{b} [K_2(b - b_0)^2 + K_3(b - b_0)^3 + K_4(b - b_0)^4] \tag{3a}$$

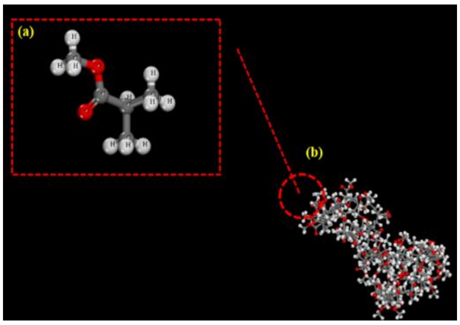

Fig. 2 (a) a monomer of PMMA (b) a polymer of PMMA with 50 chain length

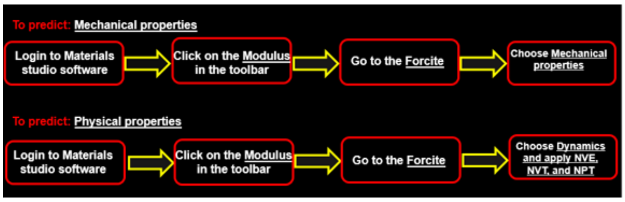

Fig. 3 Four steps to obtain mechanical and physical properties using materials studio software

$$E_{angle} = \sum_{\theta} [H_2(\theta - \theta_0)^2 + H_3(\theta - \theta_0)^3 + H_4(\theta - \theta_0)^4] \tag{3b}$$

$$E_{torsion} = \sum_{\emptyset} [V_1\{1 - cos(\emptyset - \emptyset_1^0)\} + V_2\{1 - cos(2\emptyset - \emptyset_2^0)\} + V_3\{1 - \cos(3\emptyset - \emptyset_3^0\}] \tag{3c}$$

$$E_{out-of-plane} = \sum_{\chi} K_{\chi}\, \chi^2 \tag{4}$$

V_i, H_i, K_i and ϕ_i are system dependent parameters that obtained from ab-into quantum mechanics computations. The terms of b - b_0, θ - θ_0 and $\phi - \phi_0^1$ shows the length and angle between the two neighbors' bond from the equilibrium state. θ, ϕ and χ are angles of bond, dihrealtorsion, out of plane respectively. The $E_{non\text{-}bond}$ is related Coulomb and Vander Waals potentials. The latter is expressed by the following equations

$$E_{non-bond} = E_{vanderWaals} + E_{coulomb} \tag{5}$$

$$E_{vabderWaals} = \sum_{i>j} D_0 \left[2\left(\frac{r_{ij}^0}{r_{ij}}\right)^9 - 3\left(\frac{r_{ij}^0}{r_{ij}}\right)^6 \right] \tag{6}$$

$$E_{coulomb} = \sum_{i>j} \frac{q_i q_j}{\varepsilon r_{ij}} \tag{7}$$

where D_0, q, and ε are Lenard-Jones potential, atomic electrical load and dielectric constant respectively. In this study, in order to calculate Van der Waals and Coulomb potentials, the atom-based summation with the cut-off distance of 10 A° and Evald collection method with the accuracy of 10^{-4} kcal/mol was are used. In this study, a single chain of the polymer, consisting of 50 chain length of PMMA, a widely used synthetic thermoplastic polymer has been used as a matrix as shown in Fig. 2.

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

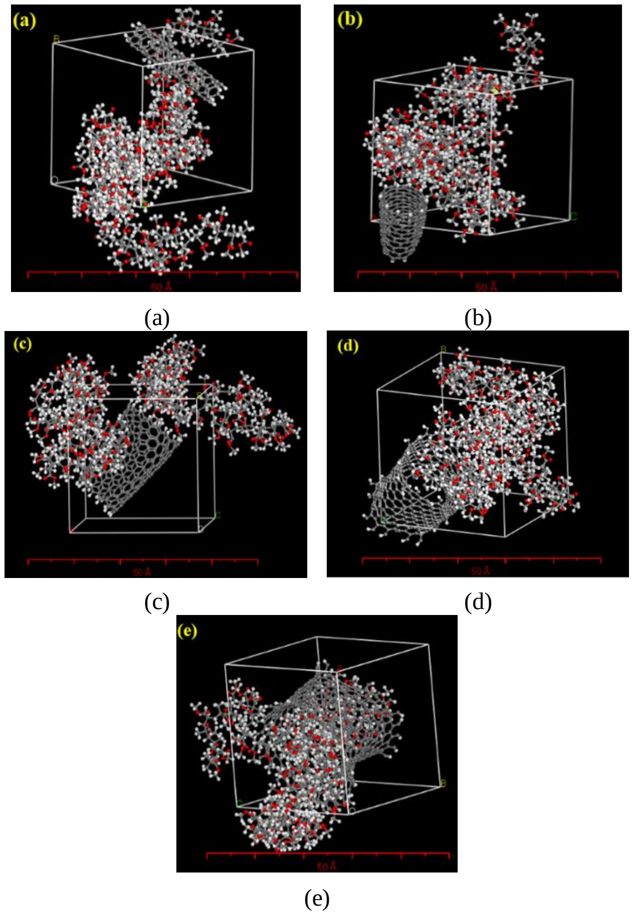

Fig. 4 Five simulated boxes with different chiralities (a) (5, 0), (b) (10, 0), (c) (15, 0), (d) (20, 0) and (e) (25, 0) using materials studio software

2.2 Simulation methodology

In this section, the effect of the diameter of SWCNTs 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 considered to be 8 gr, and the weight of the polymer (PMMA) is 6 gr. All molecular details of five case studies including type of SWCNTs, inner radius, temperature, numbers of atoms, and lattice dimensions have been shown in Table 1.

Fig. 5 illustrates the schematic of simulated nanocomposites by MDs method for obtaining physical and mechanical properties.

Table 1 Details of five case study for simulated nanocomposites boxes

Rolling procedure	SWCNT type	Inner radius (A°)	Temperature (K)	No. of atoms	Lattice dimensions (A°)
armchair	(5,0)	3.91	300	1614	26.4× 26.4×26.4
armchair	(10,0)	7.83	300	1724	27.4× 27.4×27.4
armchair	(15,0)	11.74	300	1834	28.3× 28.3×28.3
armchair	(20,0)	15.66	300	1970	29.1× 29.1×29.1
armchair	(25,0)	19.57	300	2054	29.9× 29.9×29.9

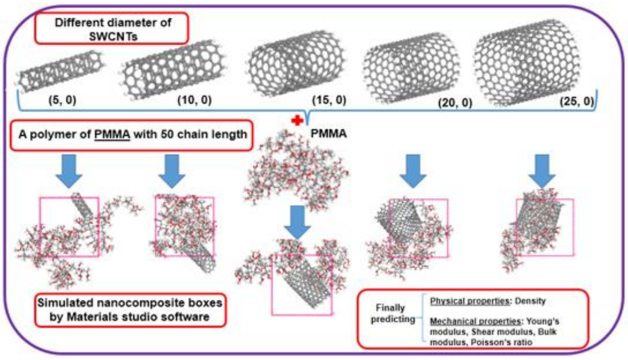

Fig. 5 Schematic of nanocomposite boxes that simulated by materials studio software

3. Result and discussion

3.1 Results of MDs for pure materials

To verify the overall results, first the properties of the pure materials are examined. The mechanical and physical properties of pure materials (SWCNTs and PMMA) are shown in Table. 2 by following the steps that mentioned above (Fig. 3). Table 2 is shown the comparison of mechanical and physical properties of (SWCNTs and PMMA) with molecular dynamics modeling and laboratory analysis. There is a good agreement between the molecular dynamics modeling and laboratory analysis.

3.2 Diagram of radial distribution function

One of the significant quantities to evaluate the equilibrium validation of the system in molecular dynamics is the radial distribution function (RDF). The RDF reports the mass distribution of the system over atomic distances, and is expressed by Eq. (8).

$$g(r) = \frac{\rho(r)}{\rho} = \frac{\langle N(r \pm \frac{\Delta r}{2}) \rangle}{\Omega(r \pm \frac{\Delta r}{2})} \frac{1}{\rho} \tag{8}$$

In this respect, the density of the number of atoms in the shell to the radius (r) in the volume and ρ is the density of the number of atoms in the total volume of the system.

To accurate the simulations RDF diagram and its equation have been obtained and added in Eq. (8). Moreover, for obtaining the mechanical and physical properties, we observe molecular atomic interactions until the simulation box reaches equilibrium. After equilibrium the simulated box, the results are predicted correctly. It is worth mentioning compass force field helps to reach this equilibrium. For solids (composites), the RDF at distances as shown in Fig. 6 must converge to the value of 1. It is a measure of the equilibrium of a solid atom's system. In this article, the RDF diagram of all five nanocomposites is obtained, but to reduce number of figures, the RDF of last nanocomposite presents as follows

Table 2 Comparison of mechanical and physical properties of pure (SWCNTs, PMMA) using between MDs method and laboratory analysis

Mechanical, physical properties	MD	Laboratory	% error between simulation and lab analysis (%)
Comparison of mechanical and physical properties of (SWCNTs) between MDs modeling and laboratory analysis			
Density (g/cm^3)	1.30	1.39 Laurent *et al.* (2010)	6.47
Young's modulus (GPa)	270	277 Tarfaoui *et al.* (2016)	2.52
Poisson's Ratio	0.30	0.32 Tarfaoui *et al.* (2016)	6.25
Comparison of mechanical and physical properties of (PMMA) between MDs modeling and laboratory analysis			
Density (g/cm^3)	1.15	1.18 Liu *et al.* (2019)	2.54
Young's modulus (GPa)	2.98	3.0 Mousa *et al.* (2000)	0.66
Poisson's Ratio	0.38	0.4 Mousa *et al.* (2000)	5

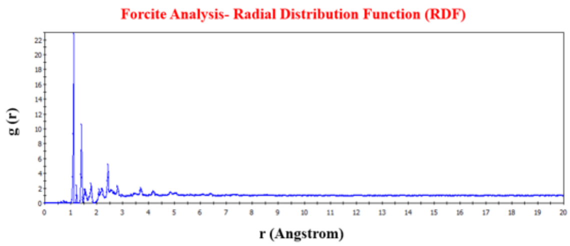

Fig. 6 Radial distribution function of atoms convergence to the number 1

3.3 Prediction of mechanical and physical properties

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. 7. The longitudinal Young's modulus is calculated 3.7, 5.1, 6.3, 7.9

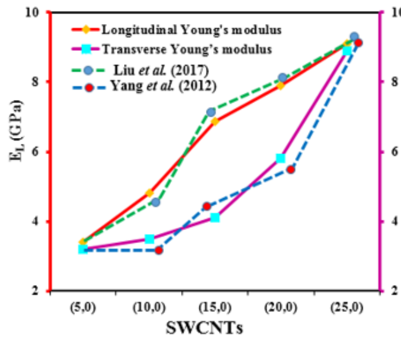

Fig. 7 Comparison between the results of the present work and the other literature (Liu *et al*. 2017, Yang *et al*. 2012) for longitudinal and transvers Young's modulus (SWCNTs-PMMA)

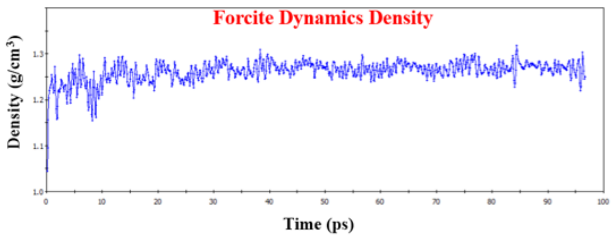

Fig. 8 Density diagram armchair SWCNTs (25, 0) mixed with PMMA

Table 3 Details of significant mechanical and physical properties of five case study for simulated nanocomposites

SWCNTs type	Density (g/cm^3)	Poisson's ratio	Shear modulus (GPa)	Bulk modulus (GPa)	E_L (GPa)	E_T (GPa)
(5,0)	0.81	0.27	4.20	2.90	3.7	3.3
(10,0)	0.83	0.28	4.29	3.30	5.1	3.8
(15,0)	0.97	0.28	5.05	3.78	6.3	4.1
(20,0)	1.04	0.28	5.09	4.26	7.9	5.9
(25,0)	1.25	0.30	6.03	5.08	9.5	9.1

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 twice increase. Also, Fig. 7 shows the comparison between the results of the present work and the other literature (Liu *et al*. 2017, Yang *et al*. 2012) for longitudinal and transvers Young's modulus (SWCNTs- PMMA). It is seen that there is a good agreement between them.

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. 8 the density was predicted approximately 1.25 g/cm^3.

To validate the simulation results, the 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.

$$C_{ij}(GPa) = \begin{bmatrix} -6.2881 & 0.5504 & 3.8897 & 1.1397 & -0.6569 & -0.6992 \\ 0.5504 & -8.8962 & -6.6375 & -4.2861 & 0.7676 & 0.4550 \\ 3.8897 & -6.6375 & -6.6422 & -1.3783 & 1.6240 & -0.3777 \\ 1.1397 & -4.2861 & -1.3783 & 1.5629 & 3.3594 & 3.0916 \\ -0.6569 & 0.7676 & 1.6240 & 3.3594 & 1.2339 & -2.1884 \\ -0.6992 & 0.4550 & -0.3777 & 3.0916 & -2.1884 & 1.16108 \end{bmatrix} \quad (1)$$

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 3 and shows with increasing of CNTs diameter, all mechanical and physical properties increase.

4. Conclusions

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.

- Predicting the effect of SWCNTs diameter on mechanical and physical properties of five cases was simulated by materials studio software.
- Physical properties enhance with increasing of SWCNTs diameter
- Mechanical properties increase due to high Young's modulus of SWCNTs
- With increasing of SWCNTs diameter, longitudinal Young's modulus from (5, 0) to (25, 0) becomes approximately 3 times more than (5, 0).
- With increasing of SWCNTs diameter, transverse Young's modulus from (5, 0) to (25, 0) becomes approximately 2 times more than (5, 0).
- With increasing of SWCNTs diameter, shear modulus from (5, 0) to (25, 0) becomes 1.43 times more than (5, 0).
- With an increase in the diameter of SWCNTs, Poisson's ratio from (5, 0) to (25, 0) becomes 1.1 times more than (5, 0).
- 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.

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