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Molecular dynamics simulation of the mechanical properties of CNT-polyoxymethylene composite with a reactive forcefield

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ABSTRACT

Carbon Nanotubes (CNTs) are potential additives to polymeric materials as they can enhance the mechanical, structural, and electronic properties of the resulting polymeric composite. However, the improvement of different properties is not always guaranteed and the results usually depend on the specific polymer used, along with the quality and quantity of CNTs used in the polymer composite. In this work, a reactive force field (ReaxFF) is applied to perform molecular dynamics (MD) simulation to determine the change in mechanical properties of single-walled carbon nanotube (SWCNT)-reinforced Polyoxymethylene (POM) composite. We have varied the diameter of CNTs from 0.542 to 1.08 nm keeping the temperature constant at room temperature (300 K) and observed a significant change in the resulting mechanical property. Volume fraction of CNT and temperature are also varied and the results are presented through a stress–strain plot. After that, our Molecular Dynamics (MD) simulation result of CNT is compared with existing literature for code validation. Dependence of mechanical property on the interaction energy, fracture mechanism, and reasons behind it are discussed elaborately. It is clear from the results that the use of SWCNT in the polymer matrix of POM significantly improves the mechanical property of SWCNT-reinforced POM composite.

1. Introduction

In 1991 a revolution in the field of nanomaterial was started with the introduction of carbon nanotubes (CNT) by Iijima [1] as CNT has excellent structural, mechanical, and electronic properties and became a focus of considerable research [2–6]. Due to the properties of having extremely high tensile strength and Young's modulus, it has become a potential reinforcement for structural and multi-functional composites and can increase strength and stiffness in many folds compared to typical carbon fibre-reinforced polymer composites [7].

Ajayan et al. [8] conducted one of the first studies about polymer/CNT composite using the arc discharged method to create multi-wall carbon nanotube (MWNT) and then dispersed randomly in a liquid epoxide-base resin by the mechanical mixing. Although polymer has lightweight and low cost, it has less tensile strength. But mixing a small percentage of CNT with it significantly increases the tensile strength of the polymer composites [9–13]. So, this mixing needs to be done carefully as it is already well known that the strength and stiffness of the fibre-reinforced polymer composite critically depends on the interfacial bonding between the polymer matrix and fibre. High fibre–polymer interfacial bonding results in high composite strength and stiffness in exchange of low composite toughness [14]. Carbon nanotube has a high aspect ratio, so large areas are available for load transfer. Now, it is clear that to take the advantage of novel property like extremely high Young's modulus or stiffness of CNT it is very essential to have an efficient load transfer between the polymer matrix and the nanotubes. This is why preparing a polymer matrix with SWCNT as reinforcement has become challenging as the dispersion of CNTs in the polymer matrix [15], improper alignment of CNT in the polymer matrix, and weak interface adhesion between the polymer matrix and CNT can significantly decrease the performance [16].

Now in most cases, CNT/polymer composite is prepared through in situ polymerisation, mechanical mixing, solution mixing, melting mixing, or solid mixing process. [16]. Due to these difficulties molecular mechanics (MM) and molecular dynamics (MD) simulation has become more and more popular among researchers for investigating CNT–polymer interface, reinforcement mechanisms in CNT–polymer composite systems specially in polymer resin [17]. MD simulations have been applied satisfactorily to predict the elastic properties of CNT–polymer composites. In 2003 MD simulation is used by Frankland et al. to represent the stress–strain behaviour of polyethylene–CNT composites where CNT is loaded mechanically in both the longitudinal and transverse directions [18]. Mahboob et al. [19] used MD simulation to investigate the effect of stone wales defect on the mechanical properties of composites reinforced with SWCNTs. Tahreen and Masud determined Young's modulus, bulk modulus, shear modulus, and compressibility of single-walled carbon nanotube (SWCNT)-reinforced polyethylene (PE) using molecular dynamics (MD) simulation which satisfactorily reproduced experimental results [20]. Kamal et al. investigated the mechanical behaviour of carbon fibre-amine functionalised multiwall

carbon nanotube/epoxy composites and determined Young's modulus, poison ratio, and validated their work with experimental results [17]. Later on, they performed a Pull-out simulation of interfacial properties of amine-functionalised multi-walled carbon nanotube epoxy composites and developed an artificial neural network (ANN) model to develop a nonlinear relationship between input–output data [21]. Four aforementioned studies used the compass force field which is suitable for condensed phase application for its hybrid approach of both ab initio and empirical methods but cannot represent the construction and destruction of chemical bonds in the simulation systems. In addition, breaking stress/strain of composites cannot be predicted by compass and it can only predict stress–strain curves in the harmonic region [22]. This limitation can be overcome by using a reactive force field like ReaxFF [23]. So later on, Xiong et al. modelled CNT-reinforced polyethylene (PE) composite with an interfacial covalent bonded interaction and used MD simulations to determine mechanical property where they used *ReaxFF* which is spatially developed for hydrocarbon and successfully reproduced the experimental result of Young' modulus of 1000 GPa for CNT [24]. Zaminpayma studied the interaction between polythiophene (PT)/ polyethylene (PE)/poly(*p*-phenylenevinylene) (PPV) and CNTs using MD simulation and determined the effect of temperature, diameter, and polymer type on interaction energy using ReaxFF [25].

ReaxFF is a multi-body potential and has been developed based on the concept of bond order which ensures a smooth transition of the energy between different molecules and uses the geometry-dependent charge calculation scheme to calculate polarisation effects and redistribution of partial atomic charges perfectly when the molecule or cluster of atoms changes its shape [23,26]. This force field has successfully optimised the trade-off between the accuracy of large-scale MD simulation and the computational expenses by establishing a bridge between quantum chemical (QC) and empirical force field (EFF) which attracts many researchers to use ReaxFF to predict the interaction of different hydrocarbons [27] and polymer–CNT composite [28,29], and this is the reason for using this force field to model our CNT–polyoxymethylene composite and predict the interaction between them.

Polyoxymethylene (POM) is a high-performance engineering plastic resin with high mechanical strength, high crystallinity, good abrasion resistance, and excellent solvent resistance. Thermal stability and the electrical conductivity can be increased with the addition of CNT, but this will decrease the crystallinity of the polymer. The polyoxymethylene (POM)–CNT can be used in different fields like anti-electrostatic, conductive, and electromagnetic interference shielding fields. Plastic particles with a perfect surface finish can be produced from the moulded POM composite filled with CNTs compared to conventional carbon fibre [16]. So CNT–POM composite may find application in manufacturing elements that work under variable load conditions as well as precision machine parts as polyoxymethylene has high dimensional stability, fatigue, wear resistance, and good sliding properties [30]. This is the reason why researchers have shown their interest in determining the mechanical property of CNT–polyoxymethylene where both single-wall CNT and multi-wall

CNT are used [31–34], but no research has been conducted yet using molecular dynamics to determine the properties of CNT–polyoxymethylene.

In the present work, we use a reactive force field (ReaxFF) which accounts for the van der Waals interaction, covalently bonded interaction, and the electrostatic interaction in the interface of the nanocomposite to conduct molecular dynamics simulation to explore the impact of the interfacial covalent-bonded interaction on the mechanical properties of carbon nanotube (CNT)-reinforced polyoxymethylene (POM) composite. We also studied the influence of CNT diameter, CNT volume fraction, and temperature on the interaction energy and after that, we computed stress–strain curves of CNT–POM composites to calculate Young's modulus and extracted the breaking stress/strain point of composites. Our investigation revealed that volume fraction and diameter play a major role in changing properties where the dependence of properties on temperature is less significant. A sharp drop in the interaction energy between CNT and POM is observed between 400 and 500 K temperature which is discussed with appropriate reasoning.

2. Simulation method

2.1. Force field (ReaxFF)

Different valance terms like angle, torsion (see Equation (1)), etc. used in ReaxFF can smoothly go to zero with the breaking of bonds as they are defined in terms of the same bond order and use a general relationship between bond distance and bond order as well as between bond order and bond energy which helps it to perform proper dissociation of bonds to separated atoms. In addition to this, ReaxFF has Coulomb and Morse (van der Waals) potentials to describe nonbonded interactions between all atoms (no exclusions). The parameters used in ReaxFF were derived from quantum chemical (QC) calculations on bond dissociation and reactions of small molecules plus the heat of formation and geometry data for a number of stable hydrocarbon compounds. A good description of these data is provided by ReaxFF as it has developed a bridge between quantum chemical (QC) and empirical force field (EFF)-based computational chemical methods which allow it to simulate the system containing thousands of atoms [23].

In general, the reactive force field ReaxFF calculates the total energy of the system from various partial energy contributions [23], which is

$$E_{system} = E_{bond} + E_{over} + E_{under} + E_{val} + E_{pen} + E_{tors}$$
$$+ E_{conj} + E_{vdWalls} + E_{coulomb}, \qquad (1)$$

where E_{bond} is the bond energy of nanosystem, E_{over} and E_{under} are the bond energy penalty of the atom over coordination and under coordination, respectively, E_{val} denotes the valence angle energy of nanosystem, E_{pen} is the angle penalty energy of the atom over coordination and under coordination, E_{tors} is the torsion angle energy of nanosystem, E_{conj} is the contribution of conjugation effects to the molecular energy, $E_{vdWalls}$ denotes nonbonded van der Waals interactions energy of nanosystem, and $E_{coulomb}$ is the coulomb interaction energy

Table 1. Comparison of Young's modulus with literature data.

Investigations	Young's modulus (GPa)
Present work	1260
Krishnan et al. [Experimental] [36]	900–1700
Salvetat et al. [Experimental] [37]	800 ± 410
Qiang et al. [Morse Potential][39]	840 ± 20
Bao WenXing et al. [REBO and LJ potential] [38].	935.805 ± 0.618

of nanosystem. The fundamental assumption in ReaxFF is that the bond order between two atoms is directly related to the bond length or interatomic distance which is not the case always and to fix this issue E_{over} as well as E_{under} is introduced. In spite of correcting the original bond order, it is possible to remain some over coordination in the system and a penalty of E_{over} is added to fix this issue. On the other hand, to take into account the effect of coordination due to resonance E_{under} is introduced. In our model, we do not have E_{pen} as energy contribution as there is no atom sharing two double bonds. Detail explanation about the energy contribution and all the parameters used in the above formulae can be obtained from [23] which also contain the detail value about the hydrocarbon parameters used for our MD simulation in the recent work.

To validate ReaxFF used in our study, we have taken armchair (6,6) carbon nanotube with a length of 4.92 nm and a diameter of 0.815 nm. ReaxFF is used to define the interaction between carbons. The system is minimised and then deformed to calculate stress and strain from which Young's modulus is obtained.

The obtained results for CNT are in a good agreement with experimental results except some small discrepancies and can be explained as a result of using different diameter CNTs and also the presence of some defects in the experimental samples which is reported by Kamal et al. [35] that defects in CNT significantly decrease the modulus of CNT. Krishnan et al. [36] used the thermal vibration of CNT, and Salvetat et al. [37] used an atomic force microscope on two ends clamped nanotubes. On the other hand, Bao WenXing et al. [38] and Qiang et al. [39] used molecular dynamics to predict different types of armchair CNTs with varying length and diameter and all of the results are very close to the result obtained by our simulation. So, the result indicates the effectiveness and accuracy of ReaxFF (Table 1).

2.2. Molecular model and MD simulations

At first, we have generated a single chain of polyoxymethylene and CNT crystal then packed the polymer chain around the SWCNT. Visual Molecular Dynamics (VMD) [40] is used to convert the initial generated model into Large-Scale Atomic Molecular Massively Parallel Simulator (LAMMPS) compatible file and post-processing. Then the final molecular dynamics simulation is carried out in LAMMPS.

A picture of the unit cell of the polyoxymethylene (POM)/CNT composite used in the current study is shown in Figure 3 from different perspectives (Figure 1).

The interfacial intermolecular distance controls interfacial C–C covalent bond so, in our work, CNT–polyoxymethylene nanocomposite interfacial bond is attained by eradicating inter-molecular distance.

A constant integration time step of 0.1 fs is used during all the simulations. In the case of uniaxial tests of nanocomposite before applying the tensile load, the energy of the system is minimised at the desired temperature using the conjugate gradient algorithm. After that, Nose–Hoover style thermostat (NVT) [41] and barostat (NPT) simulations are carried out to ensure the desired temperature and zero pressure in all directions.

The uniaxial deformation is performed under NPT ensemble to control temperature fluctuations with a strain rate of $10^{11} \ s^{-1}$ $10^{11} \ s^{-1}$ from which we have generated a stress–strain curve and calculated breaking stress, breaking strain, and Young's modulus from them.

3. Results and discussion

3.1. Effect of diameter

To determine the effect of diameter change, the molecular structure of CNTs was built using three different diameters of 0.542, 0.815, and 1.08 nm where the length of the CNTs was kept constant at 4.92 nm in the middle of an amorphous simulation cell with a dimension of 3 nm × 3 nm × 4.919 nm. On the other hand, a single chain of polyoxymethylene was built having 20 repeating units containing 82 atoms, and then the polymer chain was packed into the simulation with geometry optimisation. This packing results in 51, 53, 56 chains to be
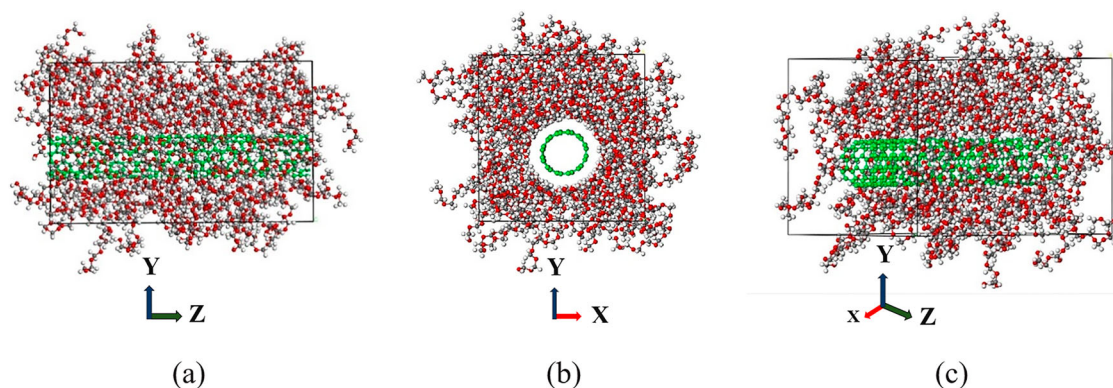

(a)   (b)   (c)

Figure 1. (Colour online) The MD model of CNT/polyoxymethylene (POM) nanocomposite, (a) side view (900 view), (b) front view (00view) and (c) lateral views (450view) (CNT carbon: green; hydrogen: white; oxygen: red and POM carbon: grey).
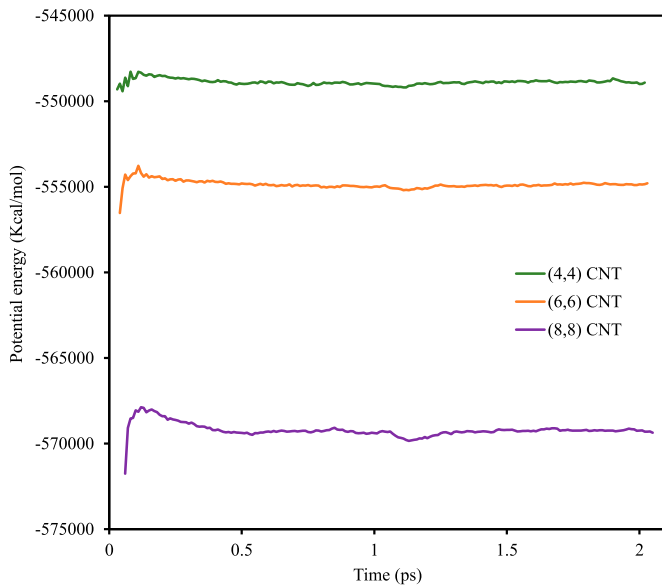
Figure 2. (Colour online) Potential energy evolution of CNT–polyoxymethylene composite for different CNT diameters during 11 ps of equilibration at 300 K.

packed randomly into the simulation cell to obtain the initial nanocomposite structure with a density of 1.42 g/cm³.

At the first stage, we studied the interaction between a CNT and a chain of the polymer. If the covalent chemical bonding is absent, the interfacial bond strength in the molecular system comes mainly from the electrostatic and van der Waals forces. The interfacial bond strength between the CNT and polymer can be measured by the interaction energy, ΔE [42] which is

$$\Delta E = E_{total} - (E_{CNT} + E_{polymer}), \qquad (2)$$

where E_{total} is the total potential energy of the system including polymer and CNT, E_{CNT} is the potential energy of the CNT without the polymer, and $E_{polymer}$ is the potential energy of th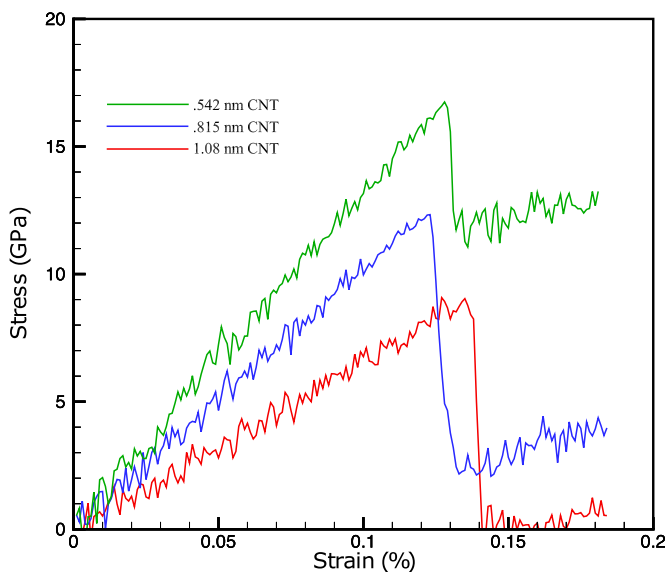e polymer without CNT. This method actually calculates interaction energy as the difference between the minimum energy of the CNT–POM composite simulation cell and the energy at an infinite separation of the polymer matrix and the nanotubes. The interaction energy is used to measure adhesion between polymer and CNT where a strong interaction energy is an indication of the strong adhesion.

Figure 2 represents the potential energy of the simulation box at a different diameter of CNT. To mimic the real-life scenario, we need to minimise the energy of the system as every stable structure remains in minimum energy. The figure indicates a sign of equilibration and a stable structure as the oscillation of the potential energy is very negligible and the fluctuations are observed in the system after 180 fs is less than 0.03%.

Figure 3 represents a stress–strain relationship used to determine breaking stress, breaking strain, and Young's modulus where catastrophic brittle failure is observed on the polymer matrix and the final load bearing observed on the graph is due to CNT fibre. Figure 4 represents the dependence of Young's modulus on the CNT radius where the increase in Young's modulus is observed by increasing CNT diameter. This phenomenon is an expected one from the interaction energy relationship calculated using Equation (2) illustrated in Figure 4. If we look carefully on the fracture mechanism presented in Figure 5, then we can observe that polymer matrix being pulled out from the CNT reinforcement keeping the CNT undeformed. So, the strength of CNT is not a critical issue here; rather interaction energy between them plays the main role in determining CNT–polyoxymethylene tensile property.

The relation between the interaction energy and the CNT radius is shown in Figure 4 where interaction energy changes from −105 kcal/mol to −649 kcal/mol with varying CNT diameter. The reason behind this can be explained as the surface contact area between the CNTs and polymer matrix increases with an increasing radius of CNTs and results in increasing
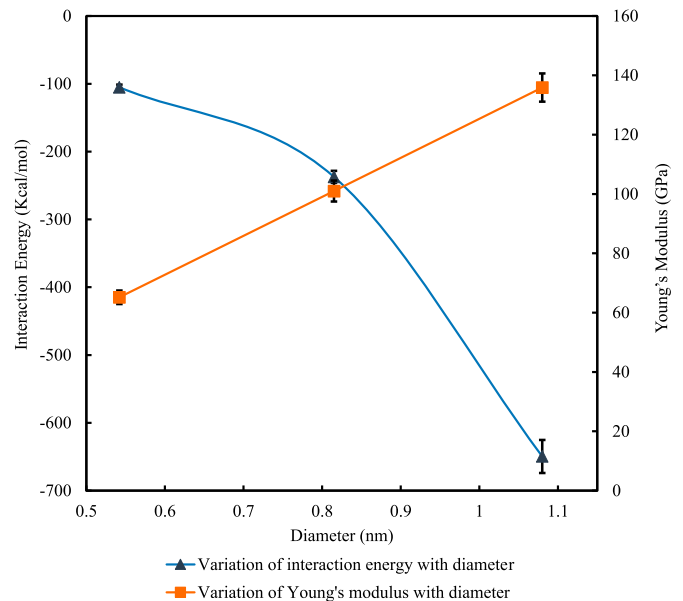

Figure 3. (Colour online) Stress–strain curve for CNT–POM composite at different CNT diameters.

Figure 4. (Colour online) Change in interaction energy and Young's modulus with respect to the diameter.
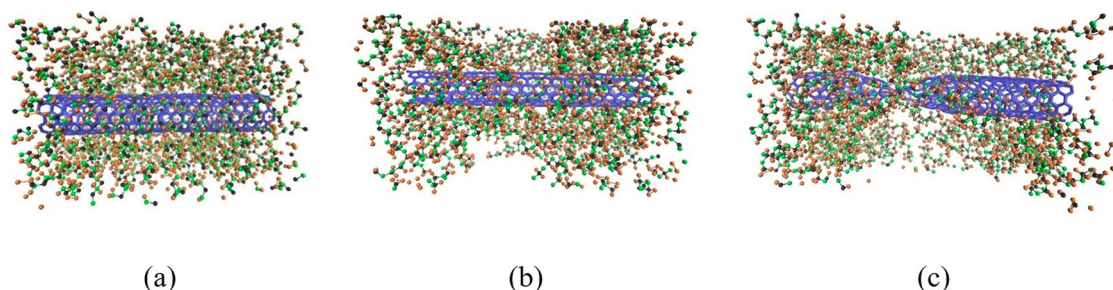
Figure 5. (Colour online) MD simulation snapshots of the atomic arrangement of (6,6) CNT–POM composite at different strain values. (a) strain = 0; (b) strain = 1.2% and (c) strain = 2.3%.

the interaction energy. But the rate of increase in interaction energy is following a decreasing (see Figure 4) trend. This is due to the large deformation of the polymer network to accommodate the large diameter CNTs. So this suggests that in spite of inserting a large diameter CNT insertion of multiple small diameter CNTs is more favourable as it will increase surface area with respect to minimal polymer deformation [43].

3.2. Effect of CNT volume fraction

The Carbon Nanotube (CNT) volume fraction plays a significant role in defining the mechanical properties of the composite. Since the polymer matrix does not penetrate the CNTs, and we use (6,6) SWNT in this purpose with a radius of 0.815 nm which can be treated as a solid beam. Therefore, the entire CNT cross-section, f_{CNT} is included as its effective volume fraction and is defined by

$$f_{CNT} = \frac{\pi \left(R_{CNT} + \frac{h_{vdW}}{2} \right)^2}{A_{cell}},$$ (3)

where h_{vdW} is the equilibrium van der Waals separation distance between the CNT and the matrix, and A_{cell} is the cross-

sectional area of the unit cell transverse to the nanotube axis. The nature of the CNT–polymer interfacial interaction drives the van der Waals separation distance and was calculated to be 0.3035 nm in the present work.

Using Equation (3) CNT volume fraction is calculated as 10.9%, 8% and 6.02% with varying the amorphous cell dimension which results in packing 53, 76 and 102 number of a polymer chain in the simulation box with a constant density of 1.42 g/cm³.

The simulation boxes are then deformed at a constant strain rate of 0.1 per ps and the results are represented as a stress–strain graph on Figure 6 which is used to calculate breaking stress, breaking strain, and Young's modulus. Figure 7 is generated after extracting values from the above to represent the variation of Young's modulus and interaction energy with respect to CNT content which represents an increasing trend of composite Young's modulus with increasing CNT volume fraction that is very similar to the result found by the previous researcher Yue et al. [44] while investigating poly{(m-phenyle-nevinylene)-co-[(2,5-dioctoxy-p-phenylene) vinylene]}- CNT composite through MD simulation. With the increase of CNT volume fraction the interaction energy between polymer matrix and CNT also increases as an increase in CNT volume
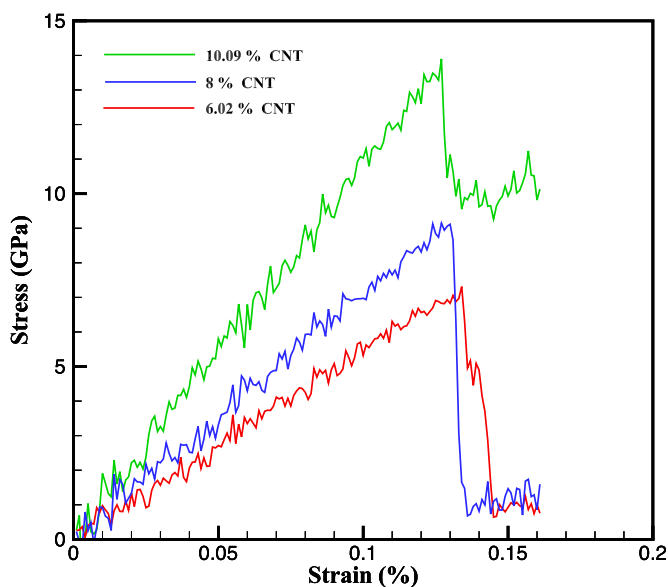

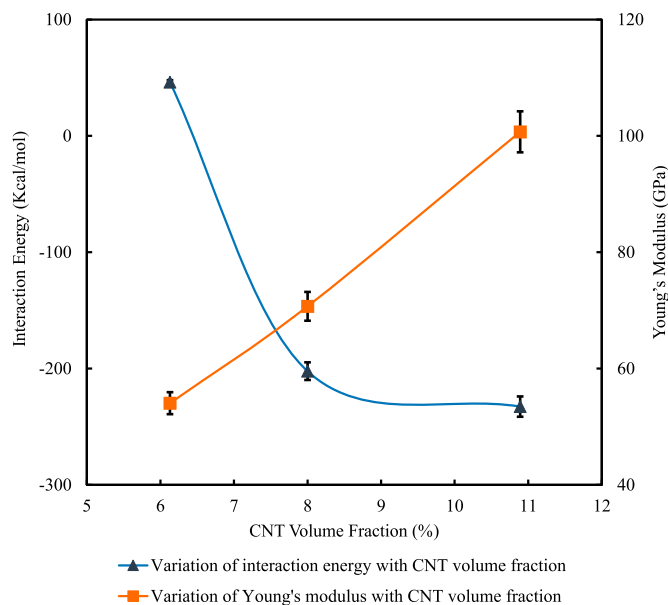**Figure 6.** (Colour online) Stress–strain curve for CNT–POM composite at varying CNT contents.

Figure 7. (Colour online) Change in interaction energy and Young's modulus with respect to CNT contents.
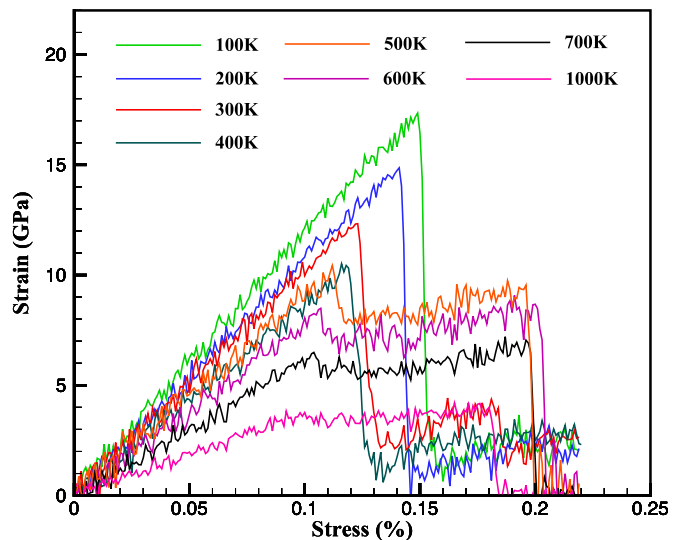
Table 2. Comparison of breaking stress and strain with changing temperature, volume, and diameter.

Temperature (K)	CNT diameter (nm)	CNT volume fraction (%)	Young's modulus (GPa)	Breaking stress (GPa)	Breaking strain (%)
300	.542	6.24	65.2 $\pm$ 1.8	13.5	9.4
	.815	10.89	101 $\pm$ 1.7	12.3	12.3
	1.08	16.7	136 $\pm$ 1.8	12.8	16.8
300	.815	6.02	54.1 $\pm$ 1.6	13.4	7.3
		8	70.7 $\pm$ 1.3	13	9.1
		10.89	101 $\pm$ 1.8	12.7	13.9
100	.815	10.89	116 $\pm$ 1.8	14.9	17.3
200			106 $\pm$ 1.5	14.1	14.9
300			101 $\pm$ 1.4	12.3	12.3
400			88.8 $\pm$ 1.7	11.9	10.5
500			89.6 $\pm$ 1.5	11.4	9
600			79.5 $\pm$ 1.9	10.7	8.6
700			62 $\pm$ 1.4	10.4	6.6
1000			37 $\pm$ 1.3	10	3.8

Figure 9. (Colour online) Stress–strain curve for CNT–POM composite at varying temperatures.

fraction gives a larger amount of polymer chain opportunity to interact with the CNT (Table 2).

3.3. Effect of temperature

To determine the effect of temperature chance CNT of .815nm diameter is used with a constant length of 4.92 nm. The amorphous cell dimension used in this purpose is the same as the above-described one and results in packing 53 polymer chain of polyoxymethylene. The simulation box is equilibrated at a varying temperature as 100K–700K and 1000K then deformed at a constant rate of 0.1 per ps. The result of MD simulations is used to determine interaction energy and a stress–strain curve is accomplished from the generated data which later on aid to determine breaking stress, breaking strain, and Young's modulus of the composite. Here Figure 10 shows a very interesting relationship between interaction energy and Young's modulus where both interaction energy and Young's modulus decrease slowly with increasing temperature except 400 and 500 K. In 400–500 K temperature interaction energy decreases dramatically that is because the glass transition of the nanocomposite falls in this range at which glassy state gets converted into the viscous state. Above 1000 K temperature, another interesting event is a drastic decrease in the interaction energy between

CNT and POM because of poor bonding between them which can be observed from Figure 8 where a clear discrepancy is visible between stable configuration of CNT–POM composite at 100 and 1000 K. In 1000 K POM chains are less compactly packed adjacent to CNT; as a result CNT is visible from yz plane of the composite resulting in poor interaction energy between them (Figure 9).

It is also observed that both interaction energy and Young's modulus decrease slightly with increasing temperature (except 400–500 K) (see, Figure 10). A similar trend is reported by Chandrani et al. [45] who reported a negligible impact of temperature and decreasing binding energy for polyacrylonitrile interactions with carbon nanotubes. We know that kinetic energy increases with the increase in temperature as a result potential energy decreases which results in decreasing interaction energy and low interaction energy means weak bonding between CNT and polymer matrix and lower modulus as bonding between CNT and polymer matrix is a bottleneck here. Another interesting observation from the stress–strain curve is that with the increase in temperature length of the steep line decreases which means a decrease in catastrophic brittle

(a)   (b)
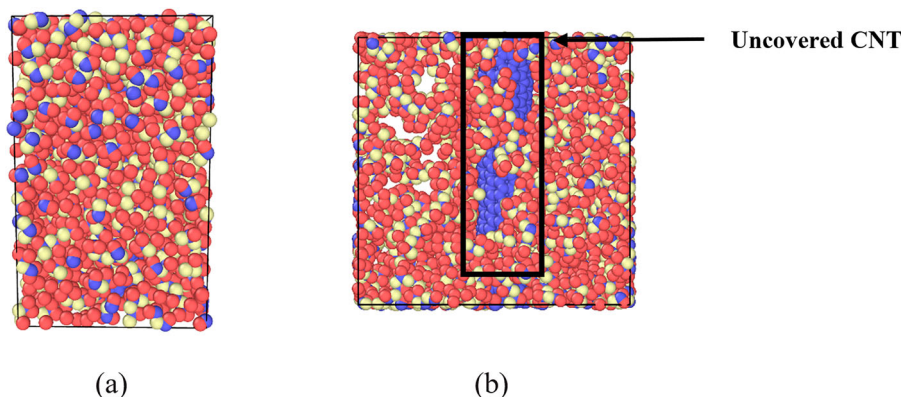
Figure 8. (Colour online) Visual representation of stable CNT–POM composite (a) at 100 K and (b) at 1000 K.
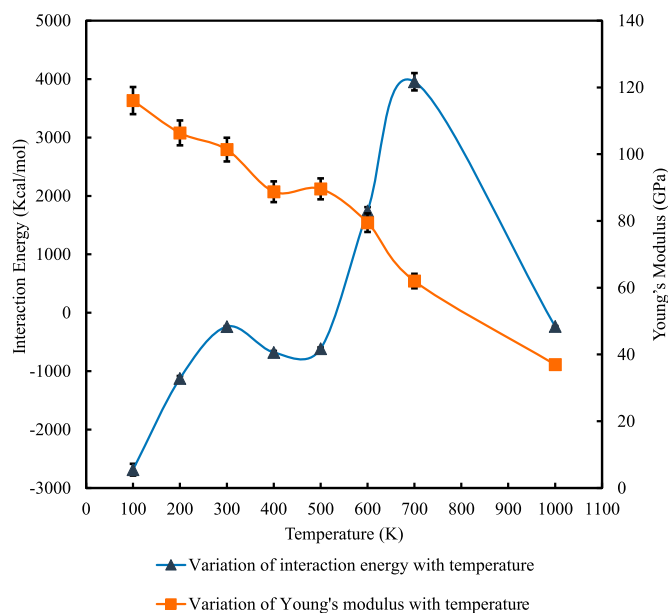
Figure 10. (Colour online) Change in interaction energy and Young's modulus with respect to temperature.

failing nature of polyoxymethylene and inclusion of some ductile nature in the matrix that is an indication of the transition from brittle to ductile with the increase of temperature.

4. Conclusions

In our study, we have used MD simulation method to investigate Young's modulus, breaking stress, breaking strain, and interaction energy with varying CNT diameter, CNT volume fraction, and temperature with a ReaxFF and it is observed that

- The temperature has a small impact on the mechanical property of the CNT–POM composite.
- CNT volume fraction and diameter plays an important role in determining the mechanical property.
- The simulation result suggested the possibility of using CNTs to mechanically reinforce the polyoxymethylene to get a novel mechanical property in both low- and high-temperature applications.

Disclosure statement

No potential conflict of interest was reported by the authors.

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References

[1] Iijima S. Helical microtubules of graphitic carbon. Nature. 1991;354:56–58.
[2] Yakobson BI, Brabec CJ, Bernholc J. Nanomechanics of carbon tubes: instabilities beyond linear response. Phys Rev Lett. 1996;76 (14):2511–2514.
[3] Che J, Cagin T, Goddard III WA. Thermal conductivity of carbon nanotubes. Nanotechnol. 2000;11(2):65–69.
[4] Treacy MMJ, Ebbesen TW, Gibson JM. Exceptionally high Young's modulus observed for individual carbon nanotubes. Nature. 1996;381(6584):678.
[5] Berber S, Kwon YK, Tománek D. Unusually high thermal conductivity of carbon nanotubes. Phys Rev Lett. 2000;84(20):4613–4616.
[6] Ebbesen TW, Lezec HJ, Hiura H, et al. Electrical conductivity of individual carbon nanotubes. Nature. 1996;382(6586):54–56.
[7] Thostenson ET, Ren Z, Chou T-W. Advances in the science and technology of carbon nanotubes and their composites: a review. Compos Sci Technol. 2001;61(13):1899–1912.
[8] Ajayan PM, Stephan O, Colliex C, et al. Aligned carbon nanotube arrays formed by cutting a polymer resin-nanotube composite. Science. 1994;265(5176):1212–1214.
[9] Thostenson ET, Chou TW. Aligned carbon nanotube composite ribbons and their production. U.S. Patent Application10/567,349, filed August 2, 2007.
[10] Ruan SL, Gao P, Yang XG, et al. Toughening high performance ultrahigh molecular weight polyethylene using multiwalled carbon nanotubes. Polymer (Guildf). 2003;44(19):5643–5654.
[11] Andrews D, Jacques AM, Rao T, et al. Nanotube composite carbon fibers. Appl Phys Lett. 1999;75:1329.
[12] Lau KT, Hui D. The revolutionary creation of new advanced materials – carbon nanotube composites. Compos Part B Eng. 2002;33(4):263–277.
[13] Andrews R, Weisenberger MC. Carbon nanotube polymer composites. Curr Opin Solid State Mater Sci. 2004;8(1):31–37.
[14] Mijovic J. Handbook of polymer–fiber composites. Polym Adv Technol. 1995;6(8):591.
[15] Pramanik C, Gissinger JR, Kumar S, et al. Carbon nanotube dispersion in solvents and polymer solutions: mechanisms, assembly, and preferences. ACS Nano. 2017;11(12):12805–12816.
[16] Wang F, Wu JK, Xia HS, et al. Polyoxymethylene/carbon nanotubes composites prepared by solid state mechanochemical approach. Plast Rubber Compos. 2007;36(7–8):297–303.
[17] Sharma K, Shukla M. Molecular modeling of the mechanical behavior of carbon fiber-amine functionalized multiwall carbon nanotube/epoxy composites. Xinxing Tan Cailiao/New Carbon Mater. 2014;29 (2):132–142.
[18] Frankland SJV, Harik VM, Odegard GM, et al. The stress–strain behavior of polymer–nanotube composites from molecular dynamics simulation. Compos Sci Technol. 2003;63(11):1655–1661.
[19] Mahboob M, Zahabul Islam M. Molecular dynamics simulations of defective CNT-polyethylene composite systems. Comput Mater Sci. 2013;79:223–229.
[20] Tahreen N, Masud AKM. Investigation of the mechanical properties of polyethylene/carbon nanotube composite by molecular dynamics simulation. Int J Nano Biomater. 2012;4(1):54.
[21] Sharma K, Sen Kaushalyayan K, Shukla M. Pull-out simulations of interfacial properties of amine functionalized multi-walled carbon nanotube epoxy composites. Comput Mater Sci. 2015;99:232–241.
[22] Sun H. COMPASS: an ab initio force-field optimized for condensed-phase applications – overview with details on alkane and benzene compounds. J Phys Chem B. 1998;102(38):7338–7364.
[23] Van Duin ACT, Dasgupta S, Lorant F, et al. ReaxFF: a reactive force field for hydrocarbons. J Phys Chem A. 2001;105(41):9396–9409.
[24] Xiong Q, Tian X, Xiong Q, et al. Atomistic modeling of mechanical characteristics of CNT-polyethylene with interfacial covalent interaction, atomistic modeling of mechanical characteristics of CNT-polyethylene with interfacial covalent interaction. J Nanomater. 2015;2015:e237520.
[25] Zaminpayma E. Molecular dynamics simulation of mechanical properties and interaction energy of polythiophene/polyethylene/poly(p-phenylenevinylene) and CNTs composites. Polym Compos. 2014;35(11):2261–2268.
[26] Buehler Markus J. Atomistic modeling of materials failure. Berlin: Springer Science & Business Media; 2008.
[27] Liu F, Hu N, Ning H, et al. Molecular dynamics simulation on interfacial mechanical properties of polymer nanocomposites with wrinkled graphene. Comput Mater Sci. 2015;108:160–167.
[28] Beese AM, Sarkar S, Nair A, et al. Bio-Inspired Carbon Nanotube–Polymer Composite Yarns With Hydrogen Bond-Mediated lateral interactions. ACS Nano. Apr. 2013;7(4):3434–3446.

[29] Saha B, Furmanchuk A, Dzenis Y, et al. Multi-step mechanism of carbonization in templated polyacrylonitrile derived fibers: ReaxFF model uncovers origins of graphite alignment. Carbon. 2015;94:694–704.

[30] Lüftl S, V PM, Chandran S. Polyoxymethylene handbook. Hoboken (NJ): John Wiley & Sons, Inc.; 2014.

[31] Yousef S, Visco AM, Galtieri G, et al. Wear characterizations of poly-oxymethylene (POM) reinforced with carbon nanotubes (POM/CNTs) using the paraffin oil dispersion technique. JOM. 2016;68 (1):288–299.

[32] Zhao X, Ye L. Structure and properties of highly oriented poly-oxymethylene/multi-walled carbon nanotube composites produced by hot stretching. Compos Sci Technol. 2011;71 (10):1367–1372.

[33] Xiaowen Zhao LYS. Preparation, structure, and property of polyoxy-methylene/carbon nanotubes thermal conducive composites. J Polym Sci B Polym Phys. 2010;48(905–912):271–280.

[34] Zhao X, Ye L. Structure and mechanical properties of polyoxymethy-lene/multi-walled carbon nanotube composites. Compos B Eng. 2011;42(4):926–933.

[35] Sharma K, Saxena KK, Shukla M. Effect of multiple stone-wales and Vacancy defects on the mechanical behavior of carbon nano-tubes using molecular dynamics. Procedia Eng. Jan. 2012;38:3373–3380.

[36] Krishnan A, Dujardin E, Ebbesen T. Young's modulus of single-walled nanotubes. Phys Rev B Condens Matter Mater Phys. 1998;58(20):14013–14019.

[37] Salvetat JP, Briggs GAD, Bonard JM, et al. Elastic and shear moduli of single-walled carbon nanotube ropes. Phys Rev Lett. 1999;82 (5):944–947.

[38] WenXing B, ChangChun Z, WanZhao C. Simulation of Young's modulus of single-walled carbon nanotubes by molecular dynamics. Phys B Condens Matter. 2004;352(1–4):156–163.

[39] Lu Q, Bhattacharya B. Effect of randomly occurring stone–wales defects on mechanical properties of carbon nanotubes using atomis-tic simulation. Nanotechnology. 2005;16(4):555–566.

[40] Humphrey W, Dalke A, Schulten K. {VMD} – {V}isual {M}olecular {D}ynamics. J. Mol. Graph. 1996;14:33–38.

[41] Plimpton S. Fast parallel algorithms for short-range molecular dynamics. J Comput Phys. 1995;117(1):1–19.

[42] Harik VM. Ranges of applicability for the continuum beam model in the mechanics of carbon nanotubes and nanorods. Solid State Commun. 2001;120(7):331–335.

[43] Gissinger JR, Pramanik C, Newcomb B, et al. Nanoscale structure–property relationships of polyacrylonitrile/CNT composites as a Function of polymer crystallinity and CNT diameter. ACS Appl Mater Interfaces. 2018;10(1):1017–1027.

[44] Han Y, Elliott JA. Molecular dynamics simulations of the elastic properties of polymer/carbon nanotube composites. Comput Mat Sci. 2007;39(2):315–323.

[45] Pramanik C, Jamil T, Gissinger JR, et al. Polyacrylonitrile inter-actions with carbon nanotubes in solution: Conformations and bind-ing as a function of solvent, temperature, and concentration. Adv Funct Mater. 2019;29:1905247.