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RESEARCH

Sliding Tribological Behavior of Carbon Nanotube/Natural Rubber Composites

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A B S T R A C T

A computational study has been made to investigate the tribological properties of carbon nanotube reinforced natural rubber composites as a function of sliding velocity at a normal loading. A three-layer model in which top and bottom layer using Iron atoms and the middle part with natural rubber matrices are constructed. Results obtained from simulations reveal that increase in sliding velocity 0.1 Å /ps to 0.11 Å /ps significantly decrease the coefficient of friction and abrasion rate. The addition of carbon nanotube to the natural rubber matrix decrease the average coefficient of friction and abrasion rate 24 % and 17 %, respectively.

1. INTRODUCTION

Carbon nanotubes (CNTs) are the boon of materials science to the scientific community. Day by day increasing use of these small nanostructures have replaced many old filler materials for the generation of durable and lightweight composites with extraordinary properties [1]. CNTs are widely used as a reinforcement for improving the mechanical, thermal and tribological properties of polymers [2-4]. The improvement depends on several parameters such as aspect ratio, size of the particle, dispersion state and the chemistry of surface that determines the interface between filler and polymers [5-7].

Natural rubber (NR) is one of the oldest rubber, but still, account for more than 40% of the total volume. Several experimental and theoretical studies have been made on the friction of rubber-based materials [8-14]. There are also numerous experimental studies which have shown the addition of fillers to polymers significantly improves their tribological performance.

Fu et al. [15] studied the mechanical and tribological properties of natural rubber (NR) reinforced carbon blacks (CBs) and Al_2O_3 nanoparticles. The studies showed the improvement in abrasion resistance and thermal stability of NR with a combination of carbon black and Al_2O_3 nanoparticles fillers. The Studies

on ZnO nanoparticle reinforced polytetrafluoroethylene (PTFE) composites shows the reduction in the coefficient of friction (COF) with increasing sliding velocity [16]. Chang et al. [17] investigated the sliding tribological properties of TiO_2 nanoparticles reinforced polyamide 66 (PA66) composites. The studies showed that nano-TiO_2 particles could remarkably improve the coefficient of friction (COF) and abrasion rate under high *pv* conditions (p = normal pressure and v = sliding velocity). At low filler loading, the reinforcement of nano-SiO_2 particles into epoxy significantly improves the tribological behavior [18]. Friction and wear behavior of polyetherimide (PEI) and polyetheretherketone (PEEK) reinforced with sub microparticles of TiO2, ZnS, graphite flakes and short carbon fiber (SCF) were studied under dry sliding condition at room and elevated temperatures [19]. The addition of conventional fillers (short carbon fiber and graphite flakes) into polymers significantly improves the load carrying capacity and abrasion rate. In addition, the sub-micro particles remarkably enhance the tribological properties at elevated temperatures. Wang et al. [20] investigated the friction and wear behavior of polyimide reinforced with nano-Si_3N_4, short carbon fiber (SCF) and graphite using a block-on-ring arrangement. The studies reveal that tribological properties of developed polymer composite greatly influenced by the sliding velocity and shows better performance under higher sliding velocities. Polymer composites filled with fibers have also studied widely by researchers as it works on the component supposed to run without external lubrication. Jacob et al. [21] used sisal/oil palm hybrid fiber as reinforcement for natural rubber. The studies conclude that the longitudinal direction gives superior mechanical properties of composites than that of transverse direction. The curing characteristics and mechanical properties of bamboo fiber reinforced natural rubber composites were studied as a function of filler loading and bonding agents [22]. The studies show adhesion between natural rubber and bamboo can be enhanced by using a bonding agent. Murty et al. [23] prepared the jute fiber reinforced natural rubber composites in the presence of silica and carbon black. Their study shows the improvement in adhesion by minimizing the resin formation and controlling it to a low molecular weight species. Sugarcane, jute, cotton, and wood fibers have also been used as potential reinforcement for improving the tribological properties of polymers [24,25].

However, experimental studies show that the carbon nanotube significantly improves the mechanical and tribological properties of the polymer in comparison to other fillers. Experimental studies of Manchado et al. [26] reveals a marked increase in the storage modulus by the addition of low content of single-walled carbon nanotubes (SWCNTs) in NR. This phenomenon was not visible with the addition of carbon blacks in equal amount. Bhattacharyya et al. [27] prepared the natural rubber composites by incorporating 8.3 % multi-walled carbon nanotubes (MWCNTs) activated by oxidation. The developed composite shows the exceptionally high tensile and storage modulus in the rubbery region at room temperature. This phenomenon was due to rigid networking effects coming from latex structure and cross-linking via functional groups on the surface of CNT and organic molecules present in the natural latex solution. The studies on polyacrylonitrile-methylmethacrylate (PAMMA) reinforced carbon nanotube copolymer nanocomposite shows the dramatic improvement in friction and wear behavior by varying wt.% addition of carbon nanotubes [28].

Further, to examine the tribological contact area which plays an important role when any new filler is introduced to the polymer. Zoo et al. [29] developed CNT reinforced ultra-high molecular weight polyethylene (UHMWPE) composites. The investigations revealed that the worn surface of the pure UHMWPE shows a broader and deeper track than that of the CNT reinforced polymer. The surface images obtained from scanning electron microscope (SEM) at higher magnifications show the locally smashed regions that indicate the changes in tribological behavior by using CNTs. In addition, the incorporation of CNT shows no changes to the internal structure of the polymer. Reinert et al. [30] studied the friction and wear behavior of CNT reinforced Nickel matrix. The experimental results show that frictional behavior is mainly influenced by the presence of CNTs in the contact zone. Zarrin et al. [31] studied the frictional behavior of CNT reinforced polymer composites at varying concentration of filler. The lowest value of friction coefficient was obtained at 0.2 % CNT concentration where it was expected a good

dispersion of nanotubes in the matrix. The friction coefficient reaches a peak value with further increase in CNTs concentration. The reason for the dramatic increase in friction was given as an increase in contact area under sliding. In addition, they reported nanohardness of the material also increases with the increase in CNTs concentration. The SEM micrographs obtained for the friction and wear test reveals that addition of CNT in polyimide (PI) composites prevents the scuffing against steel and showed much better wear resistance than pure polymer [32]. Suarez et al. [33] studied the friction and wear behavior of multiwalled carbon nanotube (MWCNT) reinforced Ni matrix. The friction test in their study was conducted at two different load regions for comparing the tribological performance. The study based on tribochemical showed the formation of oxide and carbon coating films in the samples. In their report, the developed CNT interfacial layer in the friction process worked as friction-reducing agent. The friction mechanism for low and higher loads were related to indentation depth of the dynamic counterpart and oxidation plus interfacial lubrication. The outcomes of studies showed the size of grains decreased by adding CNTs which improved the hardness, friction coefficient and wear rate. Reinert et al. [34] investigated the ways to improve the quality of metal matrix composites by employing suitable carbon nanoparticle materials. The studies proved that the grain refinement was more dependent on the agglomerate distribution within the matrix rather than on the actual agglomerate size. In addition, refinement of grains directly influenced the hardness of the materials which was also discussed in study [33]. Lim et al. [35] investigated the CNT distribution effect on tribological behavior of alumina-CNT composites from 0 to 12wt.% content. The introduction of tape casing followed by lamination and hot pressing showed the superior tribological properties.

Molecular dynamics (MD) simulation is considered as one of the most influential tool to predict the properties at the molecular level. Brostow et al. [36] proposed characterization methodology and new methods of studying static and dynamic friction. The scratch testing of polymers using molecular dynamics simulation has been studied [37]. The studies showed that the behavior of each macromolecular chain segment at each moment in time can be studied using MD simulation. Chawla and Sharma [38] developed a three-layer model to predict the friction and wear behavior of graphene oxide (GO) reinforced styrene-butadiene rubber (SBR) using MD simulation technique. Brostow et al. [39] using MD simulation studied the sliding wear behavior of a coarse-grained model of high-density polyethylene (HDPE). The increase in scratching force leads to higher penetration depths and lower recovery depths. The outcomes of the research revealed that tribological properties of polymers can be efficiently study by using the same rod for multiple sliding velocities. There are many experimental studies on the tribological behavior of polymer composites, but decidedly less at the molecular level.

Although, mostly all experimental and theoretical studies show the enhancement in tribological properties of CNT reinforced polymer composites. The mechanism of enhanced tribological properties at the atomic level when CNT used as reinforcement is given in study [40].

In this study, sliding tribological behavior of carbon nanotube reinforced natural rubber composites is studied by using molecular dynamics simulation technique. A three-layer model as described in author's previous studies has been used [38,40]. The coefficient of friction and abrasion rate are calculated at multiple sliding velocities of 1m/s to 11m/s. Further, radial distribution function and average van der Waals energy have been calculated during sliding to support the observed phenomenon. To the best of the author's knowledge, this will be the first molecular level study on the tribological behavior of CNT reinforced NR composites.

2. MATERIALS AND METHODS

2.1 Modeling of Filler

In this study, for modeling and simulation, the Amorphous Cell and Forcite module of Materials Studio (MS) 2017 software have been used. Firstly, a single-walled carbon nanotube (SWCNT) of diameter 6.78 Å and aspect ratio of 3.26 was constructed. The stress-strain curve for

the same was calculated by using a Perl script. Fig. 1, shows the stress-strain curve for an armchair (5,5) SWCNT which makes a good agreement with previous research [41].

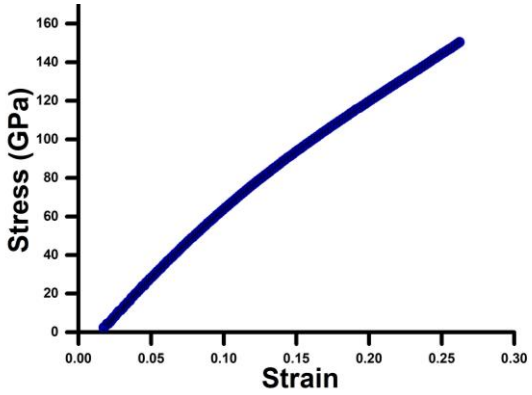

Fig.1. Stress-Strain curve of single-walled carbon nanotube (d=6.78Å).

2.2 Force Field

The selection of force field is considered as a key point of any atomistic simulation study. The force field helps in an accurate enough approximation of the potential energy surface in which the nuclei moves. The potential energy can be described as follows:

$$E_{total} = E_{valence} + E_{cross-term} + E_{non-bonded} \quad (1)$$

The valence energy term includes the bond-stretching term, bending energy and the four body terms including a dihedral bond-torsion angle term and an inversion (out-of-plane interaction) term :

$$E_{valence} = E_{stretching} + E_{bending} + E_{dihedral\,torsion} + E_{inversion} \quad (2)$$

The cross-term includes the energy changes induced by the change in the bond length and the angle changes in the surrounding atoms as given in Eq. (3):

$$E_{cross-term} = E_{bond-bond} + E_{angle-angle} + E_{bond-angle} + E_{end\_bond-torsion} + E_{middle-bond-torsion} + E_{angle-torsion} + E_{angle-angle-torsion} \quad (3)$$

The non-bonded term includes the inter- and intramolecular interactions, including Van der Waals interactions which are the induced dipole–dipole interactions (also named as London forces), the Coulomb interactions which account for electrostatic interactions and finally, hydrogen bonds (H-bonds). The non-bonded term includes the inter- and intramolecular interactions, including Van der Waals interactions which are the induced dipole–dipole interactions (also named as London forces), the Coulomb interactions which account for electrostatic interactions and finally, hydrogen bonds (H-bonds).

$$E_{non-bonded} = E_{vdW} + E_{Coulomb} + E_{H-bond} \quad (4)$$

The condensed phase optimized molecular potential for atomistic simulation studies (COMPASS) force field has been used several times for calculating the mechanical and tribological properties of polymer composites [42-46]. The COMPASS force field uses the following terms for various components of the total potential energy:

$$E_{bond} = \sum_{b} [k_2(b-b_0)^2 + k_3(b-b_0)^3 + k_4(b-b_0)^4], \quad (5)$$

$$E_{angle} = \sum_{\theta} [k_2(\theta-\theta_0)^2 + k_3(\theta-\theta_0)^3 + k_4(\theta-\theta_0)^4], \quad (6)$$

$$E_{torsion} = \sum_{\emptyset} [k_1(1-\cos\emptyset) + k_2(1-\cos 2\emptyset) + k_3(1-\cos 3\emptyset)], \quad (7)$$

$$E_{oop} = \sum_{\chi} K_2\chi^2, \quad (8)$$

$$E_{bond-bond} = \sum_{b}\sum_{b'} k\,(b-b_0)(b'-b_0'), \quad (9)$$

$$E_{angle-angle} = \sum_{\theta}\sum_{\theta'} k\,(\theta-\theta_0)(\theta'-\theta_0'), \quad (10)$$

$$E_{bond-angle} = \sum_{b}\sum_{\theta} k\,(b-b_0)(\theta-\theta_0) \quad (11)$$

$$E_{bond-torsion} = \sum_{b}\sum_{\emptyset} (b-b_0)[k_1cos\emptyset + k_2cos2\emptyset + k_3cos3\emptyset] \quad (12)$$

$$E_{angle-torsion} = \sum_{\theta}\sum_{\emptyset} (\theta-\theta_0) \times [k_1cos\emptyset + k_2cos2\emptyset + k_3cos3\emptyset], \quad (13)$$

$$E_{angle-angle-torsion} = \sum_{\emptyset}\sum_{\theta}\sum_{\theta'} k\,(\theta-\theta_0)(\theta'-\theta_0')\,cos\emptyset \quad (14)$$

$$E_{Coulumb} = \sum_{ij}\frac{q_i q_j}{r_{ij}} \quad (15)$$

$$E_{vdw} = \sum_{ij}\epsilon_{ij}\left[2\left(\frac{r_{ij}^0}{r_{ij}}\right)^9 - 3\left(\frac{r_{ij}^0}{r_{ij}}\right)^6\right] \quad (16)$$

Where:
k, k_1, k_2, k_3, k_4 = force constants determined experimentally,
b, θ = bond length and bond angle after stretching and bending, respectively,
b_0, θ_0 = equilibrium bond length and equilibrium bond angle, respectively,
ϕ = bond torsion angle ,
χ = out of plane inversion angle,
ϵ_{ij} = well depth or bond dislocation energy,
r_{ij}^0 = distance at which the interaction energy between the two atoms is zero ,
r_{ij} = interatomic distance between the atoms/molecules ,
q_i, q_j = atomic charges on the atoms/molecules
ε_0 = permittivity of free space,

This force field is implemented in the Material Studio 2017 materials modelling and simulation application package, which was used in this study.

2.3 Modeling of composite

The monomer of natural rubber (NR), 3 chains with 10 repeat units and packed molecules in a simulation cell at an initial density of 0.98 g/cm^3 have been illustrated in Fig. 2.

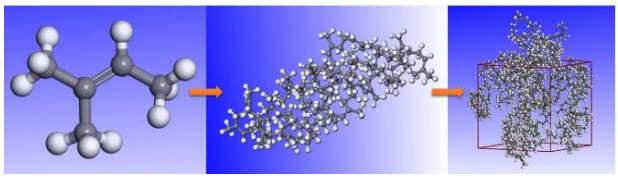

Fig. 2. (a) Natural rubber monomer (b) 3 Natural rubber chains with 10 repeat units (c) Natural rubber molecules packed simulation cell.

Firstly, an energy minimization for the developed NR matrix and CNT/NR composite has been performed using the conjugate gradient method. The convergence criteria used for this step was 1×10^{-4} Kcal/mol and 0.005 Kcal/mol/Å for energy and force, respectively. The optimized simulation cells were first heated in 20 K increments from 300 K to 500 K and then cooled back to 300 K in 20 K increments. All annealing processes were performed for the duration of 50 ps under isothermal-isobaric (NPT) ensemble. Then, to obtain the system with less residual stresses and proper density, the system was put into NPT ensemble for 2000 ps. The integration of Newtonian equations of motion was performed by Verlet velocity time integration method [47] with a time step of 1 fs. The non-bonded interactions were calculated by applying a cutoff distance of 15.5 Å. The spline and buffer widths in this study were 1 Å and 0.5 Å, respectively. The structure obtained from this step was later used for studying the tribological properties.

2.4 Modeling of the layer system

To study the friction and wear behavior of carbon nanotube reinforced natural rubber (NR), a three-layer model was constructed. The modeling methodology has been shown in Fig. 3.

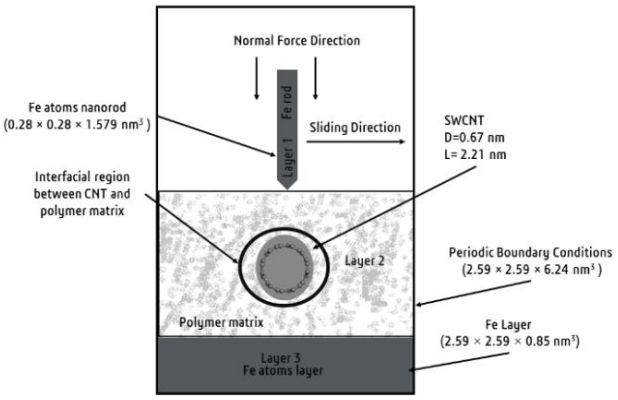

Fig. 3. Modeling strategy of pure NR matrix and CNT/NR composite for the calculation of tribological properties.

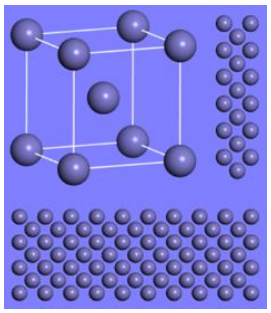

Fig. 4. Development of top Iron nanorod and bottom layer using BCC (body-centered cubic) structure of Iron (Fe).

Since Iron (Fe) is widely used as antifriction material in progressing cavity pump technology [38,40], the top and bottom layers are designed by Fe element atoms. The development strategy of Iron atom layers has been shown in Fig. 4. The three-layer model which contain the top and bottom layer of Fe (Iron) atoms in the size of 0.28 × 0.28 × 1.579 nm^3 and 2.59 × 2.59 × 0.85 nm^3, respectively. A periodic boundary condition of dimensions 2.59 × 2.59 × 6.24 nm^3 has been used for obtaining accurate results of the simulation.

2.5 Calculation of tribological properties

The developed three-layer system by using 'Build Layer' module of Materials Studio 2017 software package is illustrated in Fig. 5. The energy minimization of the layer system has been performed by using the same criteria as given in section 2.3.

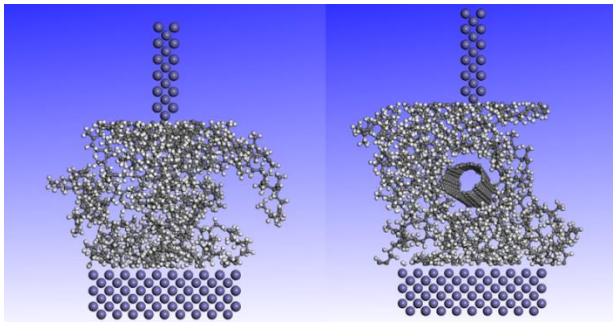

Fig. 5. The initial three-layer model of (a) pure natural rubber matrix (b) carbon nanotube reinforced natural rubber composites.

A 5-cycle annealing process at an initial temperature of 150 K and mid-cycle temperature of 300 K for 50ps was performed before sliding the nanorod to composite surface. The temperature during annealing process was controlled by using NVT (the constant volume, constant temperature) ensemble. The time step for this process was set to be 1 fs. Finally, by applying a load to the top wall (Fe rod), the relative motion was developed between the top wall and a bottom wall. A normal loading of 0.12 GPa and sliding velocities of 0.01 Å/ps to 0.11 Å/ps (1 m/s to 11 m/s) has been applied for 400 ps to all the simulations.

3. RESULTS AND DISCUSSION

To calculate the tribological properties of CNT reinforced NR as a function of sliding velocity. A series of sliding velocities with a difference of 2 m/s (0.02 Å/ps) has been applied. The trajectory of the molecules was stored and later analyzed to calculate radial distribution function (RDF) and the behavior of other responsible forces. The coefficient of friction (COF) was calculated by $\mu = \frac{F_N}{F_T}$, where μ is the COF; and F_N and F_T are normal force and friction force, respectively. The molecules moved out from the polymer matrix during the sliding process were considered as worn out molecules. The ratio of worn out molecules to the molecules of the whole polymer matrix is known as abrasion rate [45]. The obtained COF and abrasion rates of pure NR and CNT/NR as a function of sliding velocity are plotted in Figs. 6 and 7. The average values of COF for pure NR matrix and CNT/NR were obtained as 0.457 and 0.346, respectively. The addition of CNT in NR matrix shows the decrease of 24 % in the average COF. The obtained result makes a good agreement with previous experimental study [48]. The addition of CNT significantly improves the mechanical, thermal and tribological properties of polymer composites [49-51].

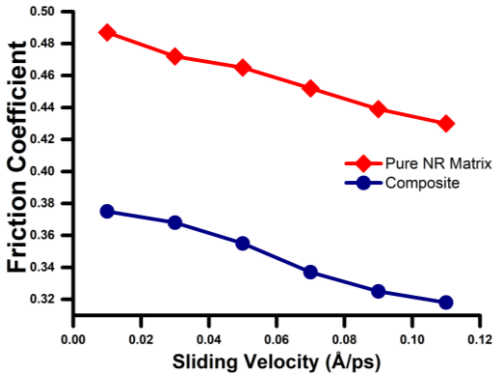

Fig. 6. Coefficient of friction with respect to sliding velocity.

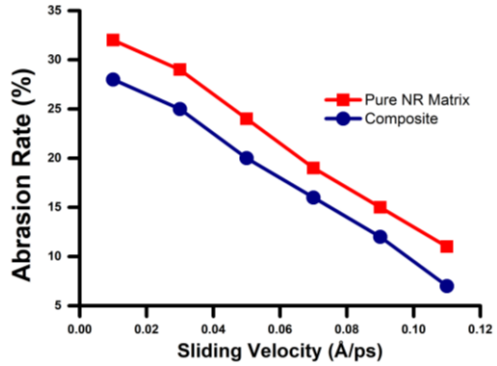

Fig. 7. Abrasion rate with respect to sliding velocity.

The strong bonding strength between carbon nanotube and styrene-butadiene rubber resist the movement of molecules towards nanorod

[40]. Many experimental and simulation studies have revealed the better load transfer, uniform stress distribution, improvement in hardness and the reduction in viscosity obtained by the addition of CNTs [52-56]. From Fig. 7 the obtained average abrasion rates values for natural rubber and CNT reinforced natural rubber are 21.7 % and 18 %, which shows a reduction of 17 % in abrasion rate by the incorporation of CNT. The increase in sliding velocity from 0.01 Å/ps to 0.11 Å/ps decreases the COF of NR and CNT/NR composites from 0.487 to 0.430 and 0.375 to 0.318, respectively. The decrease in abrasion rates from 32 % to 11 % and 28 % to 7 % under the same range of sliding velocities has been obtained. This phenomenon has also been seen in an experimental study [57]. To support the results from an atomic point of view radial distribution function of the iron atoms nanorod and NR matrices under sliding velocities from 0.01 Å/ps to 0.11 Å/ps has been calculated and plotted in Figs. 8 and 9. The average values of the radial distribution function of pure NR matrix and CNT/NR matrix decrease from 0.935 to 0.815 and 0.761 to 0.526, respectively. This leads to a phenomenon in which less polymer matrices are in contact with the iron nanorod at higher sliding velocities.

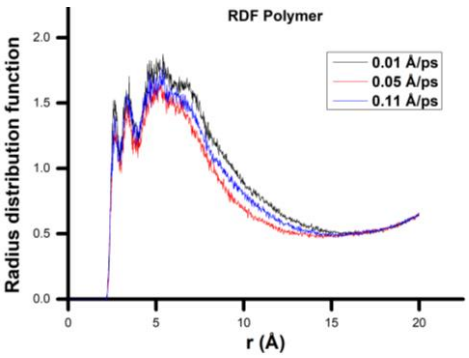

Fig. 8. Radius distribution function at different sliding velocities of Pure Polymer.

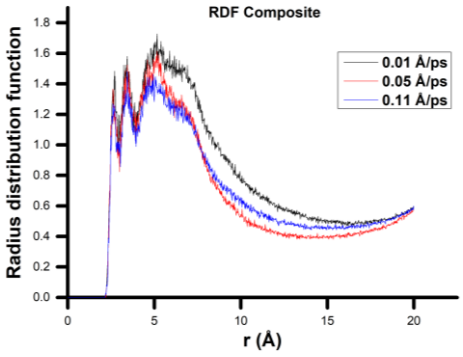

Fig. 9. Radius distribution function at different sliding velocities of CNT reinforced polymer composite.

This is because the adsorption occurs at the interface of metals and polymers [58]. On the other hand, at a low sliding velocity in the dynamics process, many molecules interact with the nanorod. Hence, from the above discussion, it can be concluded that at higher sliding velocities less polymer molecules encounter nanorod so leading to less COF and abrasion rate. Therefore, a decrease in the friction coefficients and abrasion rates are observed with increase in the sliding velocities from 0.01 Å/ps to 0.11 Å/ps.

In addition, to verify the results obtained from simulation average van der Waals energy of the pure NR matrix and CNT/NR matrix obtained during the sliding process as shown in Fig. 10. The average van der Waals energy of pure NR matrix and CNT/NR composite decreases from 53987.09 to 53850.77 Kcal/mol and 53450.23 to 52898.66 Kcal/mol, respectively under sliding velocity from 0.01 Å/ps to 0.11 Å/ps. At higher sliding velocities, it is observed that the polymer chains interact less with nanorod that leads to improve the tribological performance. The snapshots of pure NR matrix and CNT/NR composite subjected to a series of sliding velocities are shown in Fig. 11.

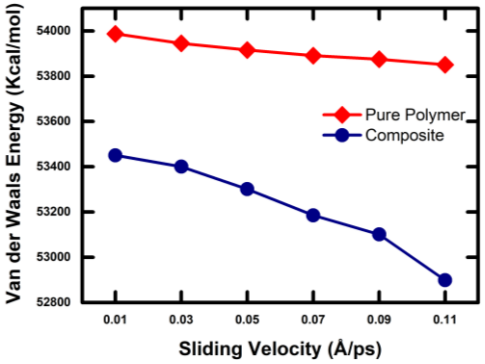

Fig. 10. Van der Waals Energy of pure polymer matrix and carbon nanotube reinforced composite.

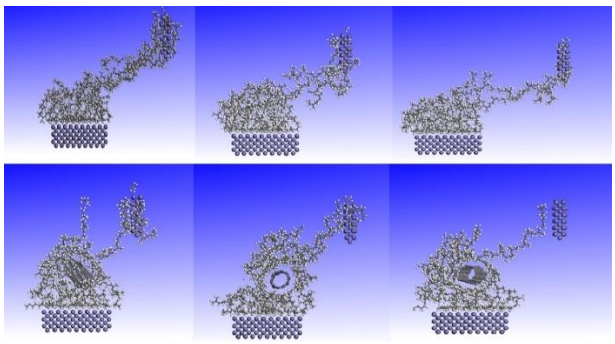

Fig. 11. Snapshots of the final states of pure polymer matrix at (a) 0.01 Å/ps, (b) 0.05 Å/ps, and (c) 0.11 Å/ps, and carbon nanotube reinforced matrix at (d) 0.01 Å/ps (e) 0.05 Å/ps and (f) 0.11 Å/ps.

From Fig. 11, it is concluded that at higher sliding velocities fewer polymer molecules interact with the Iron nanorod that improves the COF and abrasion rate. The sliding tribological behavior of polymer composites plays a vital role in various engineering applications [59,60].

4. CONCLUSION

In this study, tribological properties of CNT reinforced NR matrix have been investigated as the function of sliding velocity. The results obtained from simulations were friction coefficient, abrasion rate, radial distribution function and average Van der Waals energy. The addition of CNT into NR matrix showed the decrease of 24 % and 17 % in friction coefficient and abrasion rate, respectively. The increase in sliding velocity 0.01 Å/ps to 0.11 Å/ps decrease the friction coefficient and abrasion rate of pure NR and CNT/NR composite from 0.487 to 0.430, 0.375 to 0.318 and 32 % to 11 %, 28 % to 7 %, respectively. The obtained RDF values showed that at higher sliding velocities fewer polymer molecules interact with the Iron (Fe) nanorod. Hence, at higher sliding velocities COF and abrasion rates are low.

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