A study on the enhancement of the tribological properties of nitrile-butadiene rubber reinforced by nano-ZnO particles from an atomic view

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Abstract

In this study, three-layer molecular models of frictional pair containing nitrile-butadiene rubber matrix reinforced by nano-ZnO particle as the core and Fe layers as the counterparts are first developed. Molecular dynamics simulations are then conducted to explore the enhanced effects of nano-ZnO particle on tribological behaviors of NBR matrix. The simulation results show that the frictional coefficient of NBR matrix can be efficiently reduced by approximately 30% by incorporation of nano-ZnO particle. In order to reveal the atomic inherent mechanisms on the enhanced effects, the radius of gyration, concentration profiles, velocities distributions and temperature profiles of NBR chains are calculated and discussed in detail. Through quantitative validations of experimental works, it can be finally concluded that by incorporation of nano-ZnO particle, due to the strong vdW adsorption forces, NBR chains can be efficiently restricted around the surface of nano-ZnO particle, leading to the whole NBR matrix to perform better ability to avoid adhesive wear phenomenon, better deformation resistance, lower friction coefficients and wear loss, et al. In addition, it is also proved that the proposed molecular modeling and dynamics simulation methods can be an efficient way to provide inherent mechanisms for studying tribological properties of nano-ZnO/NBR matrix in addition to experimental works.

1. Introduction

Rubber-based materials are widely applied in a large number of engineering applications due to their outstanding mechanical, thermal and tribological behaviors [1, 2]. For instance, nitrile-butadiene rubber (NBR) is considered as the most promising material acting as the stator lining of the submersible progressing cavity pump based on its unique advantage of oil resistance [3]. In practical applications, the friction and wear phenomenon between the stator lining and metallic rotator is the key problem to deduce the life-span of the submersible progressing cavity pump leading to large economic loss [4]. Hence, in order to avoid lots of economic losses and casualties, it is of great significant to explore efficient ways and inherent mechanisms to reinforce the strength and tribological properties of NBR matrix.

In recent years, many studies were dedicated to study the improvement of the tribological properties of NBR materials by incorporation of different fillers, such as graphite, fibers, SiO₂, carbon black, et al [5–11]. Wang et al [11] studied the wear behaviors of NBR with carbon black and graphite as additives. It was found that excellent lubrication film near the wear surface of the friction pairs can be formed when good dispersion of the two reinforcements are achieved. However, it should be noted that adding excessive reinforcements have negative effects on the weight, crosslinked density and ductility of NBR matrix. Hence, based on the reinforcement system, more
Butadiene ageing resistance, facilitating the formation of network crosslinking, reducing the sulfur curing time and enhancing the thermal attentions have turned to the sulfur curing system to explore new ways to further enhance the strength and tribological properties of NBR matrix.

Zinc oxide (ZnO), as the most promising curing activator of the sulfur curing system, has the advantages of facilitating the formation of network crosslinking, reducing the sulfur curing time and enhancing the thermal ageing resistance, et al. of NBR matrix [12]. Tang, et al. [13–15] also studied the effects of different size of ZnO particles on the tribological properties of NBR matrix under dry friction conditions. The results showed that the reaction activity of ZnO particles and curing time can be enhanced and reduced respectively by continuous reducing of size of the ZnO particles. In addition, the wear rates of NBR matrix can be dramatically reduced about 75% by introduction of nano-scale ZnO particles. Li et al [16] also proved the reinforcing ability of nano-scale ZnO particles on enhancing the tribological properties of polymer matrix. They investigated the enhancing effects of different grades of the nano-scale ZnO particles on the dry tribological properties of PTFE. It was indicated that the best frictional and wear properties of PTFE matrix can be obtained when the grades of the nano-scale ZnO particles is about 15%.

Although many experimental efforts have been dedicated on the frictional and wear behaviors of NBR matrix by incorporation of nano-scale ZnO particles, lack of the inherent mechanisms on elucidating the enhancing effects have been explored from an atomic view. This is mainly due to the limitation of the small length and time scales associated with atomic level dynamics of the experimental equipment. Molecular dynamics (MD) simulations have been developed as an effective computational calculation to study the physical behaviors of different materials at an atomic level. Microscopic information and details of molecular interactions are able to be detected in addition to experimental methods. With the development of MD simulations, it has to be announced that MD simulations have been proven to be applicable to study polymer nano-composites [17]. Li et al [18] studied the improvement of tribological properties of rubber matrix reinforced by nano-SiO2 particles using MD simulations. The simulation results found that decreases of both the friction coefficient and abrasion rates of the nano-composites can be observed. The inherent mechanisms on the enhancing effects on the tribological properties of rubber composites were calculated and revealed through extracting and analyzing the atomic information obtained from the MD simulations. However, still very few MD works were carried out to study the enhanced tribological properties of NBR matrix by incorporation of nano-scale ZnO particles to the authors' knowledge.

Hence, in this study, molecular models of NBR matrix reinforced by nano-ZnO particles have been first developed. Frictional pair model containing nano-ZnO/NBR matrix and metal layers are then built. MD simulations are conducted to study the tribological behaviors of nano-ZnO/NBR matrix. Atomic profiles such as radius of gyration, temperature, atomic concentrations, et al. were calculated and discussed to reveal the inherent mechanisms on the enhanced tribological properties of nano-ZnO/NBR matrix. In addition, in order to verify the results obtained from the MD simulations, experimental works are also conducted and discussed accordingly. It is expected that the proposed MD simulation methods can be an efficient way to provide inherent mechanisms for studying tribological properties of nano-ZnO/NBR matrix in addition to experimental works to better serve the practical engineering applications.

2. MD simulations method and experimental procedure

2.1. Process of molecular modeling and simulations

For building the molecular model of nano-ZnO/NBR matrix, NBR chains in a degree of polymerization of 10 are first generated and shown in figure 1(a). The allocation ratio of the two repeat units (Acrylonitrile and Butadiene) of NBR chains is set to be 4:1. The molecular plate model of ZnO in a size of 15.6 × 15.6Å is developed and shown in figure 1(b). It is noted here that the plate model of ZnO can be shrunk into particle shape after MD equilibrations. A periodic unit cell in a size of 37.3 × 37.3 × 37.3Å is then constructed and packed with the pre–prepared NBR chains and nano-ZnO plate in a target density of 0.97 g cm−3. It has to be noted that the module of Amorphous Cell in a software of Accelrys Materials Studio (MS) is adopted in the modeling process. The NBR chains are gradually generated and filled into the unit cell by a rule of Monte Carlo style. In order to study the tribological behaviors of nano-ZnO/NBR matrix, a frictional pair model containing metal atoms as the top and bottom layers, and the nano-ZnO/NBR matrix as the middle layer is then developed. The size of the top and bottom layers is set to be 37.3 × 37.3 × 8.6 Å. Fe element is adopted since it is widely used as a counterpart in simulation training in the application of submersible progressing cavity pump [3].

To obtain a reasonable configuration in a local and global minimum energy of the frictional pair molecular model, geometry optimization tasks should be conducted. The energy and force convergence tolerances are chosen to be 0.0001 kcal mol−1 and 0.005 kcal mol−1 Å respectively. A 5-round anneal simulation is then performed under a 500 ps NVT ensemble from 300 K to 500 K to release the internal stresses in the nano-ZnO/NBR matrix. The time step during the MD simulations is set to be 1 fs. Another 500ps NVT simulations are then
followed at the temperature of 300K. Finally, the frictional process is applied to the upper Fe atoms layer by moving the layer toward the x axis (OA) in a speed of 0.1 Å/ps for 2000 ps at a temperature of 298 K(NVT). For the purpose of studying the enhancing effects of ZnO particles on the tribological properties of NBR matrix, another frictional pair model without incorporation of ZnO into NBR matrix is constructed. The final structures of both the nano-ZnO/NBR and Non-ZnO/NBR models are shown in figures 1(c) and (d) respectively.

It is worthy to be announced that during all MD simulations, COMPASS potential, which is the first ab initio force-field is adopted [19]. It was proved that this molecular potential is applicable to obtain accurate calculations of a wide range of polymer materials [20, 21]. Methods of the Andersen thermostat [22] and Berendsen barostat algorithm [23] are applied for the temperature and pressure conversion. The Ewald summation method [24] with an accuracy of 0.001 kcal/mol is adopted to calculate the electrostatic interactions. In addition, 12.5 Å is applied for the cutoff distance of Van der Wall (vdW) nonbond interaction.

2.2. Experimental procedure
In order to validate the proposed methods and results provided by MD simulations, experimental efforts are conducted accordingly. For the materials preparation, nitrile-butadiene rubber purchased from Lanzhou Petrochemical Company with 18% content of acrylonitrile is adopted as the masterbatch. The nano-scale ZnO particles in average sizes from 10–15 nm provided by Shandong Xingya New Materials Co., Ltd are adopted. It has to be noted here that we try to select the minimum sizes of the ZnO particles to emphasize their nano-scale
effects in the macro experimental investigations. In addition, other processing aids, such as sulfur, stearic acid, carbon black, accelerator benzothiazole disulfide, tetramethyl thiuram disulfide, magnesium oxide, softener dioctyl phthalate are adopted during the preparation of NBR matrix. More detail information about the preparation of the materials are introduced in the reference [14]. Finally, block simples of nano-ZnO/NBR and Non-ZnO/NBR matrix are well-prepared for the comparison of the tribological properties. In the friction and wear experimental testing, a microprocessor controlled abrasive wear tester MPV-600 developed by Jinan Puye Mechanical and Electrical Technology Co., Ltd is adopted. Following the parameters from the MD simulations, all the dry sliding friction tests are carried out at room temperature for 600s. A linear frictional velocity of 5 m s\(^{-1}\) is adopted. After the tribological properties testing, the worn surface morphologies of rubber specimens are characterized by JSM-6360LV scanning electron microscope for further discussions.

3. Results

The frictional coefficients of both the nano-ZnO/NBR and Non-ZnO/NBR along with the MD simulation times are depicted in figure 2, respectively. From figure 2, dramatic deceasing trends of the frictional coefficients of both the two matrices can be observed in the early stage of the frictional processes. This large fluctuation phenomenon can be explained that due to the initial instable configurations of the molecular models, larger error can be occurred inevitably. Nonetheless, it can be clearly seen that after 150ps, the variations of the frictional coefficients of both the two matrices tend to be stable. From figure 2, the average frictional coefficient of the nano-ZnO/NBR matrix is obtained to be 0.0721, which is about 30% smaller than that of the Non-ZnO/NBR matrix of 0.1029 during the stable stage of the MD frictional processes. It is indicated that after incorporation of the nano-ZnO as reinforcements, better tribological properties of NBR matrix is achieved. It can be seen that the friction generated during the friction between the rubber and the rigid body surface comes from the viscosity hysteresis on the one hand, and the adhesion caused by the direct contact between the rubber and the counterpart on the friction surface [15]. The presence of nano-ZnO strengthens the force between the rubber molecular chains in the bulk phase, weakens the mutual attraction between the rubber and the pair at the friction interface, and reduces the adhesive friction between the friction pairs. Therefore, the nano-ZnO nitrile rubber has a lower stable value of friction coefficient.

In addition, the snapshots of the final states of both the nano-ZnO/NBR and Non-ZnO/NBR matrices are provided in figures 3(a) and (b). From figure 3(a), it can be clearly seen that the Non-ZnO/NBR matrix is suffered a serious and irreversible deformation leading the whole matrix to behave a semi-fracture state. In contrast, from figure 3(b), it is shown that the NBR matrix perform a better integrity and stronger structure which is reinforced by nano-ZnO particle than that of the Non-ZnO matrix. Hence, it can be understood that the NBR chains are well-bonded around the nano-ZnO particles leading the whole NBR matrix to behave a better shear deformation resisting, fracture bridging and tribological properties.

In order to study the inherent mechanisms of the enhanced effects of nano-ZnO particles on the tribological properties of NBR matrix, the structural analysis of NBR matrices is first conducted. The gyration radius of the two NBR matrices during the MD simulations are shown in figure 4. It should be note that the radius of gyration...
is a physical index for describing the structure-related properties, which here reflects the flexibility of the NBR chain. The larger radius of gyration indicates the higher flexibility of polymer chains [25]. In the meantime, it is well acknowledged that during the process of thermodynamic motion, the extensions and curling of polymer chains can be easily formed. In the frictional process, the NBR chains are subjected to external forces leading to the thermodynamic movement of stretching and crouching. The internal friction and mechanical damping will be occurred during the stretching and crouching of the molecular chain. The internal friction and shearing force to the NBR matrix can be caused due to the viscous lag phenomenon leading to heat dissipation. Hence, higher energy dissipations can be occurred when greater values of radius of gyration are achieved, which finally weaken the mechanical, friction and wear resistance properties of NBR matrix [26]. From figure 4, it is indicated that the radius of gyration of Non-ZnO/NBR matrix (3.07) is obviously 4.2% larger than that of nano-ZnO/NBR (2.95) matrix, which reveals that the flexibility of NBR chains of Non-ZnO/NBR is higher and prone to slip with each other. It can be hence concluded that the internal friction of NBR chains are weaken by incorporation of nano-ZnO particle. It is not easy for the NBR chains to be stretched under the external stress during the frictional process.

To further verify the analysis of inherent mechanisms of the enhancing effects on the tribological properties of NBR matrix, the relative atomic concentration profiles of both the two friction pair models in the thickness direction (Z axis) is calculated and shown in figure 5. From figure 5, it can be seen that the atomic concentration of NBR chains of Non-ZnO/NBR matrix near the friction region (around 11.4 and 44.4 Å) is greater than that of the nano-ZnO/NBR matrix. Meanwhile, it can also be seen from figure 5 that in the middle region of the NBR structures (between 23 and 33 Å), the atomic concentration of the nano-ZnO/NBR matrix is 1.97, which is 3.14% greater than that of the Non-ZnO NBR matrix of 1.91. This phenomenon can be explained as followings: During the process of the frictional MD simulations, the NBR chains near the frictional interface are subjected to more intense thermodynamic movement, and a large number of NBR chains tend to accumulate around the

![Figure 3](image1.png)

(a) Shear conformation on Non-ZnO/NBR (b) Shear conformation on nano-ZnO/NBR

Figure 3. The final states of both the nano-ZnO/NBR and Non-ZnO/NBR matrices of the MD frictional simulations.

![Figure 4](image2.png)

Figure 4. The gyration radius of the two NBR matrices during the MD simulations.
frictional interface to form an adsorption layer [27]. Compared to the Non-ZnO/NBR matrix, the additional nano-ZnO particle enhances the binding force between the NBR chains due to the strong surface vDW interactions. The flexibility and thermal movements of the NBR chains are hence reduced leading the whole nano-ZnO/NBR matrix to perform a higher rigidity statement. More chains of nano-ZnO/NBR matrix are prevented to move to the Fe atom layer than that of the Non-ZnO/NBR matrix during the frictional process. Hence, it can be concluded that better ability of resistance to shear deformation and antifriction of NBR matrix can be obtained by incorporation of nano-ZnO particle. The results are in a good agreement with the radius of gyration discussed in the former section.

In order to further study the enhanced tribological properties of NBR matrix by incorporation of nano-ZnO particle, the temperature and velocity profile of NBR atoms in the thickness direction of both the two NBR matrices are shown in figures 6 and 7 respectively. As can be seen from figure 6, the average temperature of the Non-ZnO/NBR matrix is 298.94K which is about 6.57% greater than that of the nano-ZnO/NBR matrix of 280.52K. Especially near the friction interface (44.4 and 11.4 Å), the average temperature of Non-ZnO/NBR matrix is 307.51 and 326.25K, which is 12.5% and 6.6% higher than that of nano-ZnO/NBR matrix respectively. The lower temperature observed in the nano-ZnO/NBR matrix is mainly due to the existence of nano-ZnO particle, which strongly absorb the surrounding NBR chains leading less NBR atoms interact with the upper and lower Fe layers. Moreover, because of the high relative concentration of atoms on the frictional interface in the

**Figure 5.** Relative concentration profile of both the two NBR matrix during the MD frictional simulations.

**Figure 6.** Temperature distribution profiles of both the Non-ZnO/NBR and nano-ZnO/NBR matrices during the MD simulations.
Non-ZnO matrix, the thermodynamic movement of atoms in this region is more intense, which could lead to more energy dissipation and higher heat accumulations on the frictional interface. When the energy reaches a critical value, the surface materials will depart from the Non-ZnO matrix, leading to a final failure of the NBR matrix due to the process of higher energy accumulations [28]. In addition, without incorporation of nano-ZnO particle, it can be understood that adhesive wear phenomenon can be easily occurred on the Non-ZnO/NBR matrix under higher temperature leading to weak tribological properties.

Finally, the velocity distributions of both the two NBR matrices along the Z axis during the frictional processes are shown in figure 7. As can be seen from figure 7, the atomic velocities of the two NBR matrices reach their peak values near the two frictional interfaces (11.4 and 44.4 Å). The peak velocities in the upper and lower friction interfaces of nano-ZnO/NBR composites are 1.02 and 0.35 Å ps$^{-1}$, which are 11.8% and 37.1% lower than those of the Non-ZnO/NBR matrix respectively. This is due to the higher thermodynamic temperature occurred on the frictional interface of Non-ZnO/NBR matrix, resulting in more intense thermodynamic motion on the interface and greater interactions with the Fe layers. The NBR atoms of the Non-ZnO/NBR are hence more easily to be peeled off from the whole matrix than that of the nano-ZnO/NBR matrix. The presence of nano-ZnO enhances the binding force of the rubber molecular chain, maintains the integrity and rigidity of the molecular chain configuration, and restricts the thermal movement of atoms. Therefore, compared with the Non-ZnO/NBR, nano-ZnO/NBR has a lower peak of atomic velocity, indicating that the compound has better resistance to frictional shear deformation.

4. Discussion

In order to verify the results and discussions obtained from the MD simulations, experimental works are conducted accordingly. The detail information of the experimental processes is introduced in the section 2.2. The experimental results of the variation of wear loss and frictional coefficients of both the two NBR matrices are shown in figures 8 and 9 respectively. From figure 8, it can be seen that the wear loss of the Non-ZnO/NBR matrix and nano-ZnO/NBR matrices are 0.0732 and 0.021. From figure 9, it is indicated that the average frictional coefficients of the Non-ZnO/NBR matrix and nano-ZnO/NBR matrices are 0.528135609 and 0.415266917. It is indicated that the wear loss and friction coefficients of nano-ZnO/NBR matrix can be obtained to be 0.021 and 0.415. Decreases of the wear loss and friction coefficients of NBR matrix about 71.3% and 21.4% can be achieved with incorporation of nano-ZnO into the NBR matrix respectively. It can also be seen from figure 9 that the friction coefficient of the Non-ZnO/NBR compound has a time point when the friction coefficient increases over time, indicating that the wear mechanism has changed during the wear process. That is, it changes from single abrasive wear to more serious adhesive wear. That is, under the action of external shear stress, the non-ZnO/NBR friction surface undergoes more violent thermodynamic movement, and a large number of rubber molecular chains are detached from the rubber body phase, resulting in increased material wear and increased friction coefficient, while the existence of nano-ZnO restricts the thermal movement of the bulk molecular chain and maintains the rigidity of the bulk phase. Therefore, the nano-ZnO/NBR compound has a small amount of wear, and the friction coefficient with time curve remains basically stable, showing
excellent tribological properties. The enhanced friction and wear properties of nano-ZnO/NBR matrix obtained from the experimental works are in a good agreement with the results produced by MD simulations.

In addition, the SEM images of the morphologies of the worn surfaces on the Non-ZnO/NBR and nano-ZnO/NBR matrices after frictional testing are shown in figures 10(a)–(d) respectively. As can be seen in the figures 10(a) and (b), serious adhesive wear phenomena are observed obviously on the worn surface of Non-ZnO/NBR matrix. In contrast, almost no adhesion wear appears on the worn surfaces of nano-ZnO/NBR matrix (figures 10(c) and (d)) leading NBR matrix to behave stronger resistance ability. This observations are contributated to the higher temperature accumulations around the frictional surface of Non-ZnO/NBR matrix, which is in a good agreement with the calculations and discussions obtained from the MD simulations. Hence, it can be finally concluded that by incorporation of nano-ZnO particle, due to the strong vdW interactions, the NBR chains can be strongly restricted around the nano-ZnO particle leading to better integrity, resistance deformation ability and tribological properties of NBR matrix. In addition, the temperature around the frictional interface between Fe layer and NBR matrix can be reduced by incorporation of nano-ZnO particle to efficiently avoid the adhesive wear phenomenon. In addition, the proposed molecular modeling and MD simulation methods are proved to be able to explore and provide the effective inherent mechanisms of the tribological properties of nano-ZnO/NBR matrix. Hence, more works are encouraged to be extended to further study more complex modelings of nano-ZnO/NBR matrix and practical working conditions to provide more theoretical insights for better supporting for the engineering applications.
5. Conclusion

In this work, molecular models of NBR matrix by incorporations of nano-ZnO as reinforcement are built. The frictional pair models are developed by coating upper and lower Fe element layers. Shear sliding MD simulations are then conducted to study the improved effects of nano-ZnO particle on tribological behaviors of NBR matrix. Based on the MD simulation results, it is firstly indicated that a decrease of 30% of the frictional coefficient of NBR matrix can be efficiently obtained by incorporation of nano-ZnO particle. The atomic information of radius of gyration, concentration profiles, velocities distributions and temperature fields of NBR matrices are analyzed. Based on the MD simulation and experimental works, it can be concluded that by introduction of nano-ZnO particle, because of the strong vdW adsorption forces, NBR chains can be efficiently restricted around the surface of nano-ZnO particle, leading to the whole NBR matrix to perform better ability to avoid adhesive wear phenomenon, deformation resistance, lower frictional coefficient and wear loss, et al.

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Data availability statement

The data generated and/or analysed during the current study are not publicly available for legal/ethical reasons but are available from the corresponding author on reasonable request.
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