

Article

Molecular Dynamics Study on the Tribological Properties of Phosphorene/Polyethylene Composites

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Abstract: This study aimed to investigate the mechanism of phosphorene in enhancing the friction behaviors of polyethylene using molecular dynamics. A sliding model was constructed to investigate the coefficient of friction and abrasion rate of composites by applying a tangential velocity on a rigid tip. Both the size and number of layers of phosphorene had positive effects on the friction force of composites but through different mechanisms. The former was because the interaction between phosphorene and polyethylene increased with the size of phosphorene, while the latter was through influencing the thermal transport across phosphorene and polyethylene interfaces. The rate of improvement decreased with the increased layer number of phosphorene due to the fact that the phosphorene tended to congregate together and thus formed multi-layer agglomerates. The friction behavior of the composites was highly anisotropic because of the high divergence of potential-energy on the phosphorene surface. These findings have provided insights into enhancing the friction behavior of polymer filled by phosphorene.

Keywords: polymer-matrix composites; phosphorene; tribological properties; molecular dynamics

1. Introduction

In recent years, polymers have attracted increasing interest as coatings in applications with coating-specific requirements for mechanical and tribological properties due to the convenient production, outstanding mechanical properties, and excellent self-lubrication ability of polymers [1,2]. However, there are many experimental investigations on the tribological properties of pure polymers, indicating that pure polymers might not have sufficient competency for rapidly development in industrial applications. To facilitate the development of polymers in industrial applications and improve the reliability of mechanical systems, it is necessary to further improve the tribological properties of polymers because friction loss is one of the major reasons for the failure of vital engineering

components subjected to high loading. To date, many research studies have been conducted to further improve the tribological properties of polymer composites through the use of fillers, such as carbon fabric, glass fabric and glass fibers [3–6].

In the past decade, the successful isolation of single-layer graphene has aroused widespread interest in embedding two-dimensional (2D) materials in polymers as 2D materials are excellent candidates for improving the tribological behaviors of polymers [7]. Single-atom-thick 2D materials exhibit outstanding characteristics, such as unique atomic structures and supreme mechanical properties. Owing to these characteristics, single-atom-thick 2D materials can act as excellent reinforcement in polymer-based composites to enhance the tribological behaviors of polymers, e.g., coefficient of friction (COF) and abrasion rate [8]. Studies have reported that graphene, the most-developed 2D material, has a significantly positive influence on the tribological properties of polymers in view of the formation of a transfer film when sliding against the counterpart [9–12].

Recently, phosphorene (PS), a single-layered semiconductor 2D material isolated from black phosphorus, has become another prominent reinforcement for the tribological properties of polymers [13]. Compared to other 2D materials, PS has attractive properties, such as high charge-carrier mobility, in-plane anisotropy, and adjustable bandgap depending on the number of layers [14–16]. These properties, especially the significant anisotropy along different directions, enable PS/polymer composites to have a broader range of potential applications as reinforcement materials than other 2D materials [17,18]. Moreover, most 2D materials can be added to polymers to enhance their tribological and mechanical behaviors. This phenomenon is attributed to similar properties shared by 2D materials, such as a large specific surface area and a high Young's modulus. For instance, Hanlon et al. demonstrated that PS had a significant reinforcement effect on the composite modulus, strength and tensile toughness of polymer matrices [19]. PS easily agglomerated during the synthesis process of PS/polymers under ambient conditions, leading to structural degradation due to intrinsic lability of composites [20]. Therefore, few references have been made regarding the tribological properties of nanocomposites containing uniformly dispersed PS in a polymer matrix.

Molecular dynamics (MD) simulations can be used as an alternative method for predicting material properties and as a powerful tool that provides detailed insights into molecular interactions. MD simulations can help us understand the improved mechanism of PS at the atomic scale [21]. Many researchers have paid sufficient attention to the microscopic mechanisms for improving the tribological properties of composites reinforced by nanoparticles via MD simulations [22–24]. Moreover, these MD simulation results were proven to be reasonable by comparison with experimental results. From these results, it could be declared that the improved tribological properties of composites were attributed to the absorption of nanoparticles. To the best of our knowledge, however, limited MD simulations research on the PS/polymer system has been reported to date regarding the prediction of the tribological properties of polymers containing PS.

In this work, a sliding molecular model involving the PS/polymer system was constructed to investigate the enhancement behavior of PS for polymers using MD simulations. By sliding a tip over the surface of the polymers under a fixed normal force, the friction behavior of composites enhanced by PS was investigated by calculating the friction force and the abrasion rate during the sliding simulations. This study systematically investigated the effects of a variety of influential factors, including the velocity of the tip, the number of PS layers and the size of PS, on the friction behavior of composites. The anisotropy of composites was also explored by changing the velocity direction along the various lattice orientations of PS. To elucidate the reinforcement mechanism, the interfacial energy between the PS and the polymer, the temperature distribution along the direction normal to the contact surface, and the indentation depth of the tip were analyzed in this study.

2. Methodology

To explore the friction behavior of the composites containing PS, atomistic models of the composites in sliding contact with a rigid iron tip were constructed. These models are shown in Figure 1a, where

PS is highlighted in pink. The sliding simulations were realized by applying a normal load F_n and a velocity V_x to the iron tip. The normal load was modeled by applying a constant force on each atom of the tip along the z -axis. The velocity was modeled by applying an initial velocity along various directions of PS in the x - y plane. During the sliding simulations, periodic boundary conditions were applied to the system on the x - and y -axes, whereas nonperiodic and shrink-wrapped boundary conditions were applied on the z -axis.

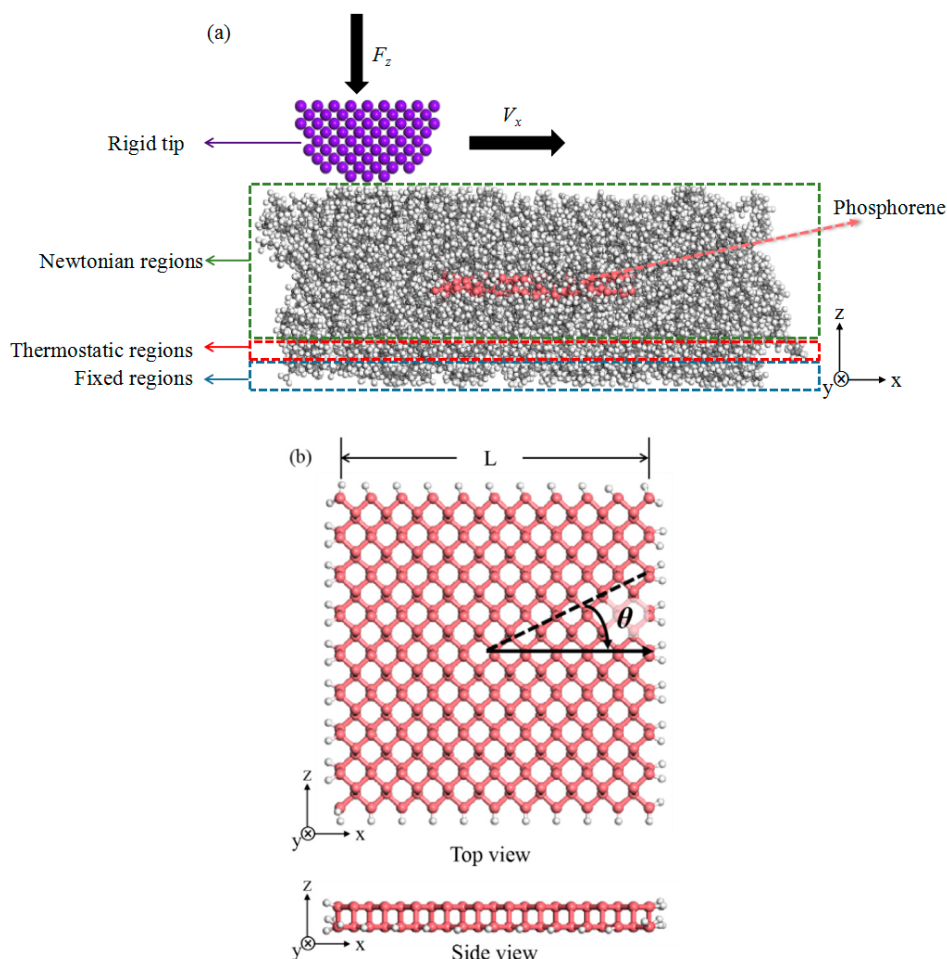


Figure 1. Conformations of molecular models of (a) the sliding interaction and (b) the phosphorene.

The tip was a hemisphere with a radius of 11.5 Å and was located at the middle of the composites on the y -axis. In addition, this tip was treated as a rigid body without geometry change during the simulations because the stiffness of the tip was much higher than that of the composites. Polyethylene (PE) with a single chain length of 30 repeating units was selected as the matrix because PE has a simple molecular structure and has been successfully applied as an anti-friction material in many fields [25,26]. Such composites are divided into three regions along the z -axis: Fixed, thermostatic and Newtonian regions. The bottom regions of the composites had a thickness of 5 Å, and the atoms in these regions were fixed at their initial positions to keep the composites static. The energy increase induced by the sliding tip was dissipated by rescaling the velocity of the atoms in the thermostatic regions to achieve the desired temperature. The atoms in the Newtonian regions are free to move under the force of their neighbors according to Newton's second law of motion.

A series of procedures were performed to obtain the initial equilibrium state of the composites. The composites were constructed by adding PS into a prepared empty cell box with a size of 3.2 Å × 41.5 Å × 37.3 Å. The armchair direction of PS was parallel to the x -direction. The PS, which is grafted by hydrogen atoms to eliminate the unsaturated effect, is shown in Figure 1b. The PE chains could

then be filled in this cell to a predetermined density via a Monte Carlo manner. The structure was relaxed until the differences in total energy and force between two adjacent time steps were less than 1.0×10^{-4} kcal/mol and 5×10^{-3} kcal/mol/Å, respectively. The temperature of the composites was set to increase from 300 K up to a desired value, which was higher than the melting point of the composites. The next relaxation was performed to eliminate the residual stress in the system under a pressure of 1 atm. After this relaxation, the system was subjected to a cooling process to obtain the equilibrium state of the composites at 300 K. Periodic boundary conditions were applied in all three directions.

The large-scale atomic/molecular massively parallel simulator (LAMMPS) was used to carry out all MD simulations. The interactions between atoms were described by the ab initio polymer consistent force field (PCFF), which had the same functional form as the condensed-phase optimized molecular potentials for atomistic simulation studies (COMPASS) force field [27,28]. The PCFF has shown a good ability to integrate organic and inorganic molecular systems and has been broadly applied to explore the tribological properties of polymer-metal systems [29,30]. The PCFF is composed of two parts, as follows:

$$E_{\text{total}} = \sum E_{\text{bond}} + \sum E_{\text{non-bond}} \quad (1)$$

where $\sum E_{\text{bond}}$ and $\sum E_{\text{non-bond}}$ are the bond and non-bond interactions of atoms, respectively. Details of the PCFF have been provided in previous reports [27,28,31]. The LJ 9-6 potential was used to describe the van der Waals (vdW) interactions between like-atom pairs. For unlike-atom pairs, a 6th order combination law was used to calculate the parameter. Both the cut-off distance of van der Waals (vdW) and Coulomb interactions were 12.5 Å, which was smaller than half of the shortest length of the simulation box. The timesteps were set as 1 fs, and visual molecular dynamics (VMD) software was used for their molecular visualizations [32].

A constant load F_n (200 pN) was applied to the tip before the sliding process to relax the whole system at 300 K for 100 ps. A stable contact was formed between the tip and the composites within this relaxation. Upon relaxation, an initial velocity V_x (2, 5, 7.5, 10 and 12.5 Å/ps) was added to the tip for a certain amount of time in the friction simulations, keeping a fixed total sliding distance (100 Å). PS with different sizes was generated by uniformly expanding the dimension of the PS in its zigzag direction to $L = 10, 20, 30, 40$ and 50 Å, whereas the dimension in the armchair direction of the PS was unchanged. In the case with different numbers of PS layers, the PS stacks in a direction perpendicular to the PS in-plane surface, i.e., A-A stacking mode. Note that the 0-layer PS represented the pure PE matrix without PS. When simulating different sizes of PS and numbers of PS layers, the direction of V_x was along the x -axis. Moreover, the anisotropy of the composites were studied by changing the friction angle from 0° to 180° with an incremental angle of 30° . In these simulations, the size and number of layers of PS were always set to 15 Å and 1 layer, respectively, and the velocity V_x was set to 10 Å/ps. The total number of PE chains was fixed at 102 for each case.

During the friction simulations, the force undertaken by the tip along the x -axis was calculated, and the friction force was set to the average of this force over 100 timesteps. Moreover, the abrasion rate was calculated by dividing the numbers of worn atoms by the number of total atoms of PE [12], wherein the worn atoms were defined as those removed from the substrate [33]. It has been confirmed that the friction behavior of a material is significantly influenced by the temperature at the contact surface [34]. To shed light on this enhancement mechanism, the atoms of composites in the Newtonian domain were divided into multiple strips along the z -axis, and each strip was calculated to obtain the temperature distribution. Furthermore, the indentation depth of the tip before the friction simulations acted as an indicator to evaluate the dependence between the hardness and friction of composites.

3. Results and Discussion

3.1. Friction Behavior

The friction force with different numbers of PS layers during the sliding process under $L = 40$ Å and $V_x = 10$ Å/ps is plotted in Figure 2. The friction force dramatically increased at the beginning of the

sliding simulations. After the friction force reached a maximum value (i.e., a maximum static force), the friction force sharply dropped and then stabilized with certain fluctuations, leading to a stick-slip friction mode. However, the periods of this stick-slip pattern were not clear because polymers do not have lattice constants [35]. As the number of PS layers increased from 0 to 5, the maximum static force decreased. Furthermore, the average friction force during the stick-slip process (indicated by the black dashed line in Figure 2) exhibited a similar trend to that of the maximum static force.

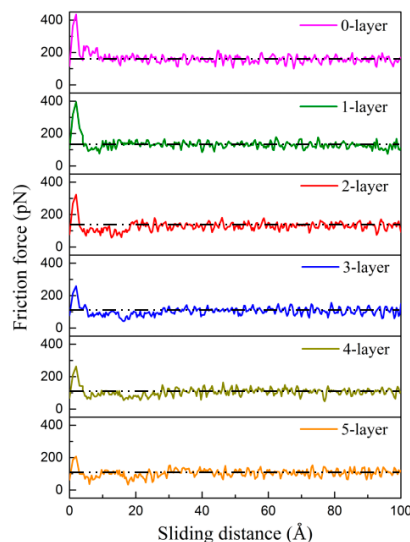


Figure 2. Friction force with different numbers of phosphorene layers during the sliding process under $L = 40 \text{ Å}$ and $V_x = 10 \text{ Å/ps}$.

To discuss the effect of PS content on the friction behavior of composites, the friction force with different numbers of PS layers and sizes of PS during the sliding process under $V_x = 10 \text{ Å/ps}$ was calculated, and the results are shown in Figure 3a. The friction force was approximately linearly proportional to the size of PS regardless of the number of PS layers. The friction force also decreased as the number of PS layers increased. However, the rate of enhancement decreased with an increasing number of PS layers and even tended toward zero when the number of PS layers exceeded a critical value, suggesting that PS with a higher number of layers might not have equivalent had enhancement as PS with a lower number of layers. These results were quite close to the earlier experimental observations, which indicated that the decreasing rate of enhancement was attributed to bulk black phosphorus in the polymer matrix formed by the agglomeration of PS [20,36]. The enhancement mechanisms of the size of PS and the number of PS layers on the PE matrix were different, as discussed in Section 3.2.

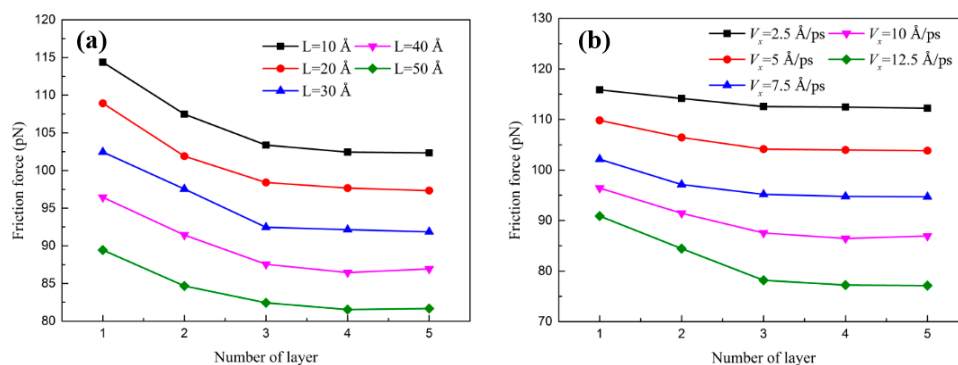


Figure 3. Friction force with (a) different numbers of phosphorene (PS) layers and sizes of PS during the sliding process under $V_x = 10 \text{ Å/ps}$ and (b) different numbers of PS layers and tip velocities during the sliding process under $L = 40 \text{ Å}$.

In addition to the PS content, the friction conditions, such as velocity, also had a significant influence on the friction behavior of materials. The friction force with different numbers of PS layers and tip velocities during the sliding process under $L = 40 \text{ \AA}$ is shown in Figure 3b. In the case of the constant velocity, the friction force showed a nonmonotonic dependence on the number of PS layers accompanied by a drop in the enhancement rate. Moreover, the friction force decreased as the velocity increased from 2.5 to $12.5 \text{ \AA/ps}$, which was consistent with the findings reported in previous studies [37]. The effect of the number of PS layers on the friction force under high velocity was much stronger than under low velocity in terms of reducing the friction force.

As discussed in previous studies [17], the PS exhibited high friction anisotropy arising from the unique shrinking structure of PS; hence, the friction anisotropy of composites must be discussed. The effects of the friction angle on the friction force and abrasion rate of composites under 1 PS layer, $L = 40 \text{ \AA}$ and $V_x = 10 \text{ \AA/ps}$ is presented in Figure 4. The friction force and abrasion rate shared a similar pattern with respect to the friction angle. When changing the friction angle along the zigzag direction, both the friction force and the abrasion rate of the composites decreased to a minimum value. The present trend corresponded well with previous simulation studies using a tip in contact with the PS instead of with the PE matrix [18].

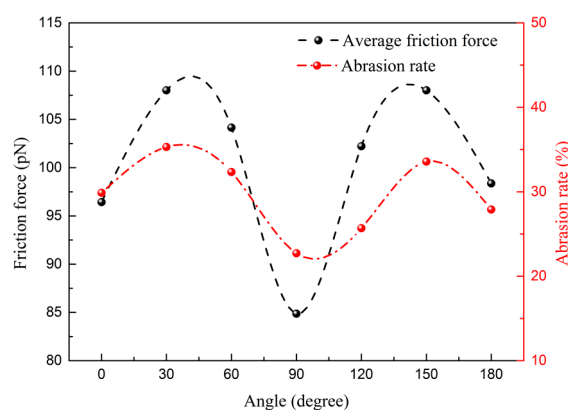


Figure 4. Friction force and abrasion rate with different friction angles during the sliding process under 1 layer of phosphorene, $L = 40 \text{ \AA}$ and $V_x = 10 \text{ \AA/ps}$.

3.2. Microstructure Evolution

The comparison between pure PE and composites with 1 PS layer and $L = 40 \text{ \AA}$ was performed to prove the enhancement effect of PS (Figure 2). The initial molecular configuration before the sliding process was first investigated. Compared to the pure matrix, an interfacial region between PS and PE was formed in the composites, as shown in Figure 5, which displays the relative contribution of carbon atoms along the z -axis. Figure 6a illustrates an image of the interfacial region between PE and PS. This phenomenon is clearly seen in this picture, which shows that the interfacial region formed on both sides of the PS.

To elucidate the improvement mechanism of the composites introduced by PS, the radius distribution function (RDF) between the iron atoms of the tip and the carbon atoms of the PE was calculated, as shown in Figure 6b. An approximately 48% decrease in average RDF values was induced by adding the PS into the polymer matrix. The influence of the PS on the friction force of polymers was attributed to the fact that fewer polymer molecules in the PS/PE composites tended to move towards the tip during the sliding process.

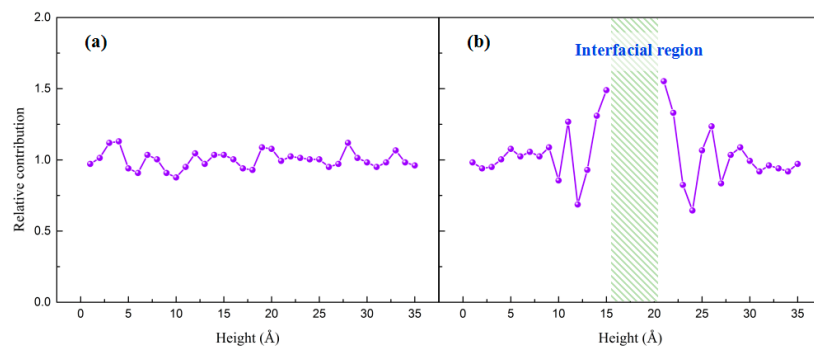


Figure 5. Relative contribution of C atoms of (a) pure polyethylene and (b) 1-layer phosphorene with $L = 40$ Å along the z-axis.

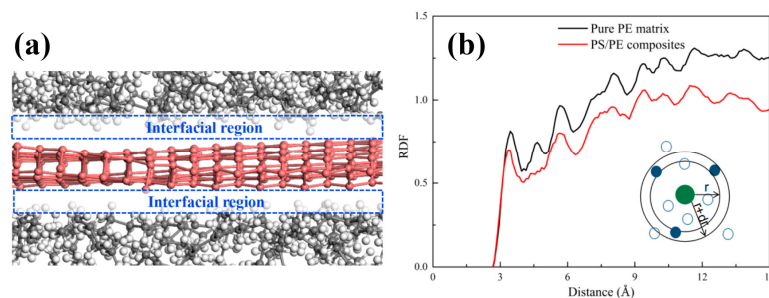


Figure 6. (a) Image of the interfacial region between polyethylene (PE) and 1-layer phosphorene (PS) with $L = 40$ Å. (b) The radius distribution function between the iron atoms of the tip and the carbon atoms of the PE.

Obviously, the interfacial interactions between PS and PE play a central key role in the friction properties of composites, which was proven by the interfacial energy changes under different PS sizes, as shown in Figure 7b. The linear relationship between the interfacial energy and the PS size was obtained from the inset image in this figure. Compared to the composites with $L = 50$ Å, the interfacial energies decreased by 40.9% and 81.3% for the composites with $L = 30$ Å and $L = 10$ Å, respectively. In general, the strong correlation between the friction force and the interaction strength observed from different sizes of PS provided insight into the mechanisms of the dependence of friction force on the size of PS. Moreover, the divergence of interfacial energy along the various lattice orientations of PS caused tribological anisotropy of composites (Figure 4). Therefore, the friction behavior of composites was related to the absorption of PS, which also proved the previous enhancement mechanism. However, the interfacial energy slightly increased as the number of PS layers increased, as shown in the inset image in Figure 7a.

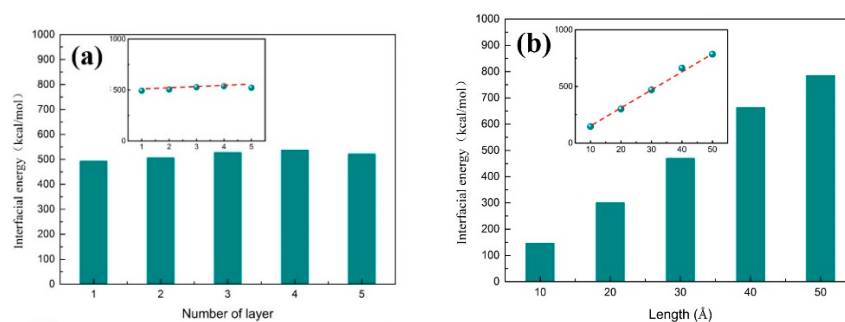


Figure 7. Interfacial energy between phosphorene (PS) and polyethylene (PE) with (a) different numbers of PS layers and $L = 40$ Å and (b) different sizes of PS with 1-layer PS.

Figure 8a shows the indentation depth with respect to different numbers of PS layers under $L = 40 \text{ \AA}$. When the number of PS layers increased, the indentation depth of the tip decreased. This decrease in indentation depth occurred because increasing the number of PS layers improved the rigidity of the composites. Therefore, under a fixed normal load F_n , the composites with a greater number of PS layers could restrict the tip from penetrating into the composites, thereby decreasing the contact area.

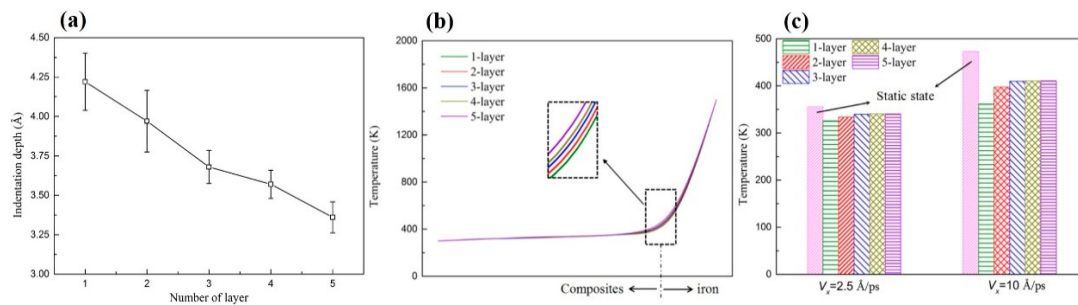


Figure 8. (a) Indentation depth with different numbers of phosphorene layers under $L = 40 \text{ \AA}$. (b) Flash temperature distribution along the z-axis at the moment of maximum static force occurrence under $V_x = 10 \text{ Å/ps}$. (c) Contact surface temperature during the stick-slip process with different numbers of PS layers and tip velocities under $L = 40 \text{ \AA}$.

Studies have reported that the interfacial adhesion strength is strongly influenced by the contact area [17]. When relative motion occurs between asperities, the temperature in the contact area rapidly increases. The temperature increases experienced under stronger interfacial adhesion strength are much higher than that under weaker interfacial adhesion strength. Such temperature increases can significantly affect the material elastic limit and plasticity, thereby influencing the friction force [38].

To explore the effect of temperature on the friction force, the flash temperature distribution along the z-axis was calculated at the moment of kinetic force occurrence, as shown in Figure 8b. The difference in temperature at the interface between the tip and the composites can explain the result that the maximum static force decreased with increasing numbers of PS layers (Figure 2). The friction force was mainly affected by the temperature at the contact surface, which agreed well with the results of previous works [34]. Figure 8c shows the temperature of the contact surface during the stick-slip process with different numbers of PS layers and tip velocities for $L = 40 \text{ \AA}$. The results showed that the number of layers influenced the interfacial temperature and subsequently the friction force (Figure 3). When the number of PS layers increased to greater than 3, the enhancement became less obvious. Compared with the interfacial temperature in the static state, the interfacial temperature during the stick-slip process for the composites with 1-layer PS decreased by 8.4% and 23.5% for $V_x = 2.5$ and 10 Å/ps , respectively, indicating that the enhancement on the contact surface temperature at low velocity was weaker than that on the contact surface temperature at high velocity.

3.3. Mechanism Analysis

In this work, the friction behavior of composites was improved by incorporating PS as reinforcement. It was reported that the friction behavior of pure PE and composites usually depends on their initial conformations [12]. In contrast to the pure matrix, an interfacial region in the composites formed between PS and PE (Figures 5 and 6). An analysis of the component of system energy showed that the potential energies of the composites were lower than that of pure PE induced by the introduction of PS. Moreover, the hardness was shown to increase as the number of PS layers increased. These phenomena lead to fewer atoms in the composites tending to move from the matrix, thereby reducing the maximum static friction force as relative motion occurred between contacting surfaces.

The interactions between the reinforcements and the matrix play a role in the friction behavior of composites and have attracted extensive studies in recent years. To explore this relationship, Li et

al. investigated the enhancement of the tribological properties of polymer composites reinforced by functionalized graphene [39]. They revealed that the enhancement of functionalized graphene was stronger than that of pristine graphene because the functionalization process improved the adhesion of nanofillers. The effect of the interactions between the reinforcements and matrix has also been proven by experimental works [11]. Our simulation results showed that the friction force depended on the size of PS. This enhancement occurs because the interaction between PS and PE becomes greater as the PS size increases, which leads to a decrease in friction. Moreover, Bai et al. evaluated the potential energy map of PS by scanning its surface in the x - y plane. The potential-profile period of the PS was consistent with its lattice periodicity, leading to the high friction behavior anisotropy of composites [17]. However, the interfacial energy slightly increased as the number of PS layers increased, whereas the friction force still decreased as the number of PS layers increased (Figure 7). This finding indicates that the enhancement mechanism of the size of PS cannot be interpreted as the enhancement mechanism of the number of PS layers (Figure 3).

The enhancement mechanism of the number of PS layers can be explained by the thermal conductivity of the composites. The atoms in the interfacial region and in the thermostatic layer are set as the hot reservoir and cold reservoir, respectively. The heated temperature induced by friction is dissipated by the cold reservoirs inside the composites. In the energy barrier theory, a high temperature reduces energy consumption in the transition from the stick process to the slip process, thereby reducing the friction force [40]. The thermal energy transport across PS and PE interfaces increases as the number of PS layers increases. However, when the number of PS layers is greater than 3, the properties of thermal conductivity remain unchanged because PS with fewer layers acts as a single material and approaches bulk properties [41]. These phenomena can explain why the friction force decreased with a decreasing rate as the number of PS layers increased (Figure 3). However, the formation of load transfer films was not found in this study, which is the main reason for reducing the friction in experimental tests [9,12]. In their tests, a high temperature at the tribological surface appeared, which may have resulted in chemical reactions, such as the formation of bonds between the tip and the composites, especially under high velocity V_x . Such chemical reactions cannot be described by using the PCFF [29]. Therefore, it is necessary to develop a more valid force field to obtain simulation results that more closely approximate experimental data.

4. Conclusions

In this paper, the reinforcement mechanism of the friction behavior of PS/PE composites introduced by PS was investigated via MD simulations. Sliding molecular models containing single- or multilayer PS were built. Based on the simulation results, PS showed a great enhancement effect on the friction behavior of PE. Compared to the pure matrix, an interfacial region at the initial molecular configuration of composites formed between PS and PE. The increasing rigidity of composites caused by the increasing number of PS layers led to decreases in the maximum static force. As the size of PS increased, the friction force of composites decreased because of the enhanced interaction between PS and PE. The friction force of the composites also decreased with increases in the number of PS layers due to the decreasing thermal conductivity of the composites. However, the thermal conductivity remained unchanged when the number of PS layers was greater than 3. The friction force and abrasion rate of 1-layered PS/PE composites shared similar trends, and both exhibited a high degree of friction anisotropy. The present work not only provides deep insight into the enhancing mechanism of the tribological properties of polymer composites containing PS but also offers guidance for synthesizing polymer nanocomposites enhanced by 2D materials with outstanding tribological properties.

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