**Impact of Interatomic Potentials on Atomic-Scale Wear of Graphene: A Molecular Dynamics Study**

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**Abstract:** Selecting an appropriate empirical interatomic potential is essential for accurately describing interatomic interactions and simulating the friction and wear of graphene. Four empirical potentials—Tersoff, REBO, AIREBO, and LCBOP—were employed in molecular dynamics simulations to study the wear process of graphene at the atomic scale. The frictional process of graphene was found to be divisible into three distinct phases: elastic deformation, plastic deformation, and wear. Using a progressively increasing load method, the critical load for each phase of graphene under four different empirical potentials was identified. Furthermore, the formation of Stone–Wales (SW) defects, bond distribution, bond breaking and healing, and wrinkle formation were analyzed in detail. Finally, a comparison was made with previous experimental results regarding friction coefficient and wear morphology.

**Keywords:** graphene; friction; wear; molecular dynamics simulation; empirical interatomic potential

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1. Introduction

Graphene possesses very high stiffness, strength, and low interlayer shear resistance [1,2]. These exceptional characteristics make it an ideal material for use in lubrication and coatings. In recent decades, tribologists have devoted great efforts to investigating the lubrication properties and potential applications of graphene in various industries [3–6]. Liu et al. [7] used a method of thermally assisted mechanical exfoliation and transfer to measure the direct sliding between graphene layers, with a friction coefficient of 0.0003 within the superlubricity regime [8]. In recent work, Li et al. [9] studied the friction behavior of graphene in various atmospheric environments. They found that graphene has a friction coefficient of 0.14–0.15 in a nitrogen atmosphere due to the destructive effects of nitrogen molecules on the ordered structures of graphene, which is much higher than the 0.06–0.07 observed in an oxygenated environment. Despite these significant nanoscale and macroscale explorations into the tribological behaviors of graphene, understanding fundamental mechanisms at an atomic level remains crucial. Especially, it is essential to reveal atomic interactions and dynamics that govern the tribological properties of graphene.

To address this, molecular dynamics (MD) simulation has emerged as a powerful tool to investigate intricate details of friction and wear processes at an atomic scale [10–14]. When performing MD simulation, one of the most important steps is choosing a potential function. Different potential functions can not only affect results quantitatively but also potentially change the behavior of a model [15]. Therefore, selecting an appropriate empirical potential is essential for accurately simulating the friction and wear of graphene. Currently, more than 40 empirical potentials are available for describing carbon systems [16]. Some of these potentials were developed specifically for pure-carbon systems, while others were designed for hydrogen–carbon, silicon–carbon, and oxygen–carbon systems. The Tersoff potential is one of the earliest and most commonly used potentials for modeling covalent systems, including carbon structures [17]. The Reactive Empirical Bond-Order potential (REBO) builds on the Tersoff potential, providing more accurate descriptions of...
bond-breaking and bond-forming processes, which are essential for simulating chemical reactions [18,19]. The Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential further extends the REBO potential by incorporating additional terms to account for van der Waals interactions and torsional forces, making it suitable for a broader range of applications, including hydrocarbons and polymers [20]. Lastly, the long-term Carbon Bond-Order Potential (LCBOP) offers a comprehensive description of both the short-range covalent interactions and the long-range van der Waals interactions, providing a balanced approach for simulating structural and mechanical properties of carbon materials such as graphene and graphite [21].

Based on factors such as computational efficiency, code availability and usage frequency, we focused on four potential functions (Tersoff, REBO, AIREBO, and LCBOP). Although these potential functions have been applied in previous studies, this is the first time that a comparative analysis of the friction and wear behavior of graphene is being conducted within a single simulation framework. In this study, we perform sliding simulations of graphene under the same conditions with four different empirical potentials to analyze the dependence of simulation results on empirical potential and provide recommendations for selecting potential functions under different frictional conditions.

2. Methods

By molecular dynamics (MD) simulations, we used four different interatomic potentials (Tersoff, REBO, AIREBO, and LCBOP) to study the friction and wear characteristics of monolayer graphene under the same sliding conditions. Our atomic model is schematically shown in Figure 1. The hemispherical amorphous carbon (a-C) tip is positioned above the single layer of graphene, which is supported by the a-C substrate. Both the tip and the substrate were cut from an a-C block prepared by a high-temperature quenching method [22]. The tip, which contains 5897 carbon atoms, has a radius of about 4.3 nm. The substrate, measuring approximately 10 nm × 15 nm × 0.8 nm in the x, y and z directions, contains 23,110 carbon atoms. Both were treated as rigid. The monolayer graphene, containing 5104 carbon atoms, has dimensions of approximately 14.1 nm in the x direction and 9.0 nm in the y direction. The periodic boundaries were applied in the x and y directions. In order to ensure that no translational motion of the graphene sheet occurs, the atoms at the graphene edges parallel to the sliding direction were fixed along the x and y directions, while remaining free to move along the z direction. Adjacent to these edges, the atoms were subjected to a Langevin thermostat to control the system temperature. The rest of the atoms in the middle of the graphene sheet could freely move along the three directions.

The Tersoff, REBO, AIREBO, and LCBOP potentials were each used to describe the C–C covalent bonds in graphene. For the other interactions, such as the van der Waals interactions between the tip, the graphene sheet, and the substrate, the 6–12 Lennard–Jones (L-J) potential was used, with the parameters \( \sigma = 0.34 \text{ nm} \) and \( \epsilon = 0.00284 \text{ eV} \) [23].

Each simulation consisted of four parts: minimizing, relaxing, loading and sliding. Firstly, the Conjugate Gradient method was performed to minimize the energy and force of the system, reaching \( 10^{-10} \text{ eV} \) and \( 10^{-9} \text{ eV/nm} \), respectively. Then, the whole system was allowed to relax for 10 ps. Afterward, the tip was pressed onto the graphene with a specific load. Under this constant load, the tip was then moved along the x direction at the specific speed for 60 ps. For each potential, we used a progressively increasing load method to determine the critical wear load. The normal load was increased by 50 nN in each simulation. In this study, the sliding speed was 100 m/s, while the system temperature was 300 K. During the scratching process, we measured the instantaneous friction force and the normal force exerted on the tip by the graphene and the substrate at the interval of 1.0 ps. The instantaneous friction coefficient was determined by dividing the corresponding friction force by the normal force. Afterward, for each simulation, the average friction force and the average friction coefficient were obtained by averaging the instantaneous values over the entire sliding distance. All simulations were performed using LAMMPS [24]. The post-processing and visualization of the data were performed in OVITO [25].
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Figure 1. An illustration of the atomistic model.

3. Results and Discussion

We investigated the frictional behavior of graphene using four empirical potential conditions: AIREBO, REBO, Tersoff and LCBOP. For each potential, we performed the sliding simulations by increasing the loads in increments of 50 nN, ranging from 300 to 900 nN, and compared the graphene responses by calculating the normal force and friction force applied to the tip. Based on different responses of C–C bonds, we categorized the scratching process on the graphene layer into three phases: elastic deformation, plastic deformation, and wear. Elastic deformation refers to situations where graphene does not undergo any permanent C–C bond breakage after the tip scratches it, or where any broken C–C bonds are subsequently repaired [26]. Plastic deformation is characterized by the appearance of Stone–Wales (SW) defects in the graphene layer [27]. Wear failure involves permanent damage or cracks [28]. Following previous studies, a C–C bond with a length exceeding 0.2 nm was considered a broken bond [29,30].

Figure 2 shows the critical normal loads for elastic deformation, plastic deformation, and wear for the AIREBO, REBO, Tersoff, and LCBOP potentials. With the AIREBO, REBO, and LCBOP potentials, graphene underwent three phases; however, the plastic deformation phase was absent when using the Tersoff potential, as shown in Figure 2. The graphene with the Tersoff and AIREBO potentials had the widest range of loads for the occurrence of elastic deformation, while the REBO graphene had the widest range of loads for the occurrence of plastic deformation. Moreover, the wear resistance of graphene with the AIREBO potential was the highest, with a critical normal load of 600 nN. In contrast, the graphene with the LCBOP potential wore out most easily, with a critical normal load of 500 nN. In the following, a detailed overview of the deformation behavior of graphene during the sliding process under the four potentials is provided.
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Figure 2. Critical normal loads of elastic deformation, plastic deformation and wear for AIREBO, REBO, Tersoff and LCBOP. Elastic deformation refers to situations where graphene does not undergo permanent C–C bond breakage after the tip scratches it. Plastic deformation is characterized by the appearance of SW defects in the graphene. Wear failure involves permanent damage or cracks. For each potential, we conducted sliding simulations with loads incremented by 50 nN, ranging from 300 nN to 900 nN, to determine the critical normal load at each phase.

3.1. Elastic Deformation Phase

During the elastic deformation phase, graphene structures undergo reversible changes without any damage [1]. For the REBO potential, graphene underwent elastic deformation when the load was less than 450 nN. During this phase, the C–C bonds in the graphene lattice were slightly strained as the tip passed over it. Taking one C–C bond (colored green) as an example, as shown in Figure 3a, its bond length increased from about 0.146 nm (i) to 0.173 nm (ii), becoming slightly distorted. As the tip continued to slide, it gradually recovered (iii), consistently maintaining the six-membered ring structure without any C–C bond breakage. In addition, the deformation behavior of graphene with the AIREBO potential is similar to that with the REBO potential, but the load range for the elastic deformation phase is 50 nN higher.

Compared to REBO, the local elastic deformation of graphene described by the LCBOP potential is more intense, involving several lattice sites. We colored three bonds to illustrate this behavior, as shown in Figure 3b. Initially, their bond lengths were approximately 0.143 nm (i). At a sliding distance of 3.5 nm, they increased to 0.18–0.19 nm (ii), and the corresponding lattices were clearly distorted. Afterward, they gradually recovered (iii).

Unlike the other three potentials, the graphene with the Tersoff potential experienced the repairable breaking of C–C bonds when the load reached 400 nN. Figure 3c depicts this phenomenon through a detailed examination of one C–C bond (colored green). Initially, as the tip approached, the bond length increased (i). The continued pressure from the tip caused the bond to break (ii), reaching a length of 0.279 nm. After the tip passed, the bond gradually recovered (iii) with a bond length of 0.147 nm.
Critical normal loads of elastic deformation, plastic deformation and wear for AIREBO, REBO, Tersoff and LCBOP. Elastic deformation refers to situations where graphene does not undergo permanent C–C bond breakage after the tip scratches it. Plastic deformation is characterized by the appearance of SW defects in the graphene. Wear failure involves permanent damage or cracks. For each potential, we conducted sliding simulations with loads incremented by 50 nN, ranging from 300 nN to 900 nN, to determine the critical normal load at each phase.

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Figure 3. Elastic deformation of graphene with (a) REBO, (b) LCBOP, and (c) Tersoff. The insets indicate the variations in length for the colored bonds at different sliding distances, and the corresponding local configuration at three sliding distances (i–iii). The colored bonds were located on the sliding path. The applied normal load was 400 nN.

Figure 4 shows the maximum bond length and the number of repairable broken bonds as a function of sliding distance during the elastic deformation phase. During the sliding process, the lengths of all C–C bonds in graphene for AIREBO, REBO, and LCBOP were calculated at each step, and the maximum one was identified. Figure 4a shows that the maximum bond length increased with increasing load for graphene of the AIREBO potential. The corresponding average values were 0.165, 0.171, and 0.172 nm for 300, 400, and 450 nN, respectively. The graphene layer using the REBO potential exhibited a similar trend, as shown in Figure 4b, but with slightly higher average values of 0.167 nm at 300 nN and 0.172 nm at 400 nN. Interestingly, as shown in Figure 4c, the maximum bond length for the LCBOP potential increased significantly compared to the AIREBO and REBO potentials, with average values of 0.179 and 0.186 nm for 300 and 400 nN, respectively. This is possibly related to the distortion of several lattice sites, as shown in Figure 3b, indicating that bonds described by the LCBOP may be softer than that by the two potentials, as Pastewka et al. showed that the bond described by the REBO potential is very stiff [31]. Additionally, as shown in Figure 4a–c, the maximum bond length varies with sliding distance, exhibiting fluctuations and lacking periodicity and symmetry. As both the substrate and the tip were made of amorphous carbon, there were certain differences in surface roughness at different positions. As a result, random vibration occurred as the tip slid over the graphene. This caused random fluctuations in the maximum bond length, with no periodicity or symmetry. For the Tersoff potential, we calculated the number of repairable broken bonds instead of the maximum bond length. As shown in Figure 4d, increasing load led to an increase in the number of repairable broken bonds from 0 at 350 nN to 2 at 500 nN. In addition, repairable bond-breaking occurred earlier at higher loads. At 400 nN, the first bond-breaking occurred at 5.5 nm, while at 500 nN, it occurred at 0.6 nm.
Figure 4. Maximum bond length of graphene as a function of sliding distance with (a) AIREBO, (b) REBO and (c) LCBOP under different loads. (d) Number of repairable broken bonds of graphene as a function of sliding distance with Tersoff under different loads.

Figure 5 demonstrates the friction behavior of graphene with the four potentials during the elastic deformation phase. As seen in Figure 5a, the friction force of graphene with AIREBO, REBO and LCBOP was significantly larger than that with the Tersoff potential under the same load. The coefficient of friction was determined by calculating the ratio between the friction force and the normal force [32,33]. Similarly, the coefficient of friction from the Tersoff potential was the smallest among the four potentials under the same load, as shown in Figure 5b. In the previous work, Qi et al. [34] used a nanoscale diamond tip to scratch mechanically exfoliated monolayer graphene onto a SiO$_2$ substrate. They obtained friction coefficients of 0.01–0.03, which are close to 0.012–0.15 from REBO, AIREBO and LCBOP at a normal load from 350 to 400 nN, but much larger than 0.004–0.006 from Tersoff. In this regard, when studying the friction of a graphene monolayer, using the Tersoff potential may underestimate the friction coefficient compared to those three potentials.

Figure 5. (a) Friction force, (b) coefficient of friction and (c) contact area as a function of normal load with AIREBO, REBO, LCBOP and Tersoff.

To explain the deviations in friction parameters between the four potentials, it is first natural to consider the contribution of contact area, as previous results have demonstrated that the larger the contact area between the tip and the substrate, the larger the generated friction [35]. The contact area of the tip with graphene was calculated by $S_{\text{contant}} = N_{\text{contant}} \times S_{\text{graphene}}$, where $N_{\text{contant}}$ is the number of atoms in contact between the tip and graphene, i.e., the number of atoms with a cutoff radius less than 0.4 nm, and...
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graphene is the area occupied by individual carbon atoms, which is about 0.0277 nm² [13]. Figure 5c shows that the contact area from the Tersoff potential was much smaller than that from the other potentials, which was consistent with the trend of both friction force and friction coefficient. This indicates that the deviations in the friction parameters between them were mainly due to the different contact areas between the tip and the graphene under the same load.

On the other hand, when comparing the friction parameters and the contact area from AIREBO, REBO, and LCBOP, the results from the REBO potential also follow the same trend. However, the contact area from LCBOP was slightly smaller than those from AIREBO, but the friction parameters exhibited contradictory results. This discrepancy is attributed to the enhancing effect of wrinkles on friction [36], which is also called the puckering effect [37,38]. The force exerted by the tip on the graphene during sliding alters the stress distribution within the graphene layer. The graphene directly beneath the tip is typically subjected to tensile stress, while the regions of graphene at the front and sides of the tip are often under compressive stress. When the compressive stress exceeds a certain threshold, the graphene undergoes deformation, resulting in the formation of wrinkles. The bonds of graphene with the LCBOP potential were easily distorted, which facilitated wrinkle formation compared to the AIREBO potential, as shown in Figure 6.

Overall, within the elastic range, the order of friction coefficients for graphene described by the four potentials under the same load is Tersoff < REBO < AIREBO < LCBOP. This result is mainly related to the contact area and is also influenced by lattice distortion and wrinkle formation.

3.2. Plastic Deformation Phase

After the elastic deformation phase, further increasing the normal load could induce the plastic deformation of graphene when using the AIREBO, REBO, and LCBOP potentials. During the plastic deformation phase, the C–C bonds rearrange locally due to the shear force, leading to changes in the microstructure. Figure 7a demonstrates the plastic deformation of graphene with the REBO potential at 450 nN. Four atoms were colored and labeled to guide the eye. When the tip approached the region with the four atoms from 4.0 nm to 5.0 nm, the C–C bonds they formed underwent minor deformation. At 5.5 nm, the deformation reached its limit. Further sliding led to the breakage of bonds 1–2 and 3–4; instead, new bonds, 2–3 and 2–4, formed at 5.6 nm. As the tip continued to move forward, these new bonds were compressed, resulting in the formation of an SW defect at 6.0 nm. We also demonstrated other three cases regarding the formation of SW defects, as shown in Figure 7b. Similarly, these defects can be considered as the 90° rotation of the bond (indicated by the red circle). For the REBO potential, although the regions where the SW defects formed were very close under 450 and 500 nN, the rotation of the different bonds resulted in the varying tilt angles of the defects. The SW defects similar to those

Figure 6. Graphene morphology with AIREBO and LCBOP during sliding under the normal load of 400 nN.
of the REBO potential at 450 nN were formed for the LCBOP and AIREBO potentials at 450 nN and 550 nN, respectively.

![Figure 7. Formation of SW defect on graphene during sliding. (a) REBO potential at 450 nN. The inset indicates the formation process. Four relevant atoms were numbered and colored in different colors. (b) REBO potential at 500 nN, AIREBO potential at 450 nN, and LCBOP potential at 550 nN. The red circles indicate the rotating bonds.](image)

Our findings using REBO, LCBOP and AIREBO confirmed that the plastic deformation of graphene could be induced by the friction force under certain loads as demonstrated by Vasić et al. [27] from the atomic force microscopy (AFM) experiments. For the Tersoff potential, however, we have not observed any plastic deformation. At this point, the Tersoff potential may be less accurate than the other potentials. Although it seems the formation of SW defects has not damaged the graphene layer with any voids or cracks, they could raise the sliding energy barrier locally and thereby increase the friction force, which has been extensively studied [39,40].

3.3. Wear Phase

Wear failure of graphene often refers to the breakdown of graphene due to its interactions with counterparts, which mainly consists of damage and rupture. As shown in Figure 2, the graphene with the AIREBO potential exhibited the highest wear resistance, while the graphene with the LCBOP potential wore out the most easily. To explain this difference for different potentials, we can analyze the bond length distribution within the contact area under relaxing and loading conditions, as shown in Figure 8.

Following the previous work [30], a C–C bond with a length larger than 0.16 nm was defined as a long bond. Before loading, most bonds had a bond length of around 0.14 nm for AIREBO, REBO, and LCBOP, while for Tersoff, most bonds had a bond length of around 0.145 nm, as shown in Figure 8. After loading, a few long bonds emerged. In our previous work, it was found that long bonds have a significant influence on the wear resistance of graphene [30]. To quantitatively describe them, the total proportions of long bonds under three different loads are shown in the figure. For each potential, the total proportion of long bonds increased with the load. For the AIREBO potential, the graphene had the fewest long bonds under the loads from 700 nN (1.62%) to 900 nN (3.24%), as shown in Figure 8a. In contrast, for the LCBOP potential, the graphene had the longest bonds under the loads from 700 nN (2.91%) to 900 nN (4.69%), as shown in Figure 8c. The total proportion of long
bonds for the other two potentials (REBO and Tersoff) lies between those of AIREBO and LCBOP, as shown in Figure 8b,d. These proportions clearly explain why the wear resistance of graphene follows the order LCBOP < Tersoff = REBO < AIREBO.

We also calculated the number of breaking bonds in the graphene layer during the sliding process. As shown in Figure 9a, the number of breaking bonds in the graphene with AIREBO increased with the sliding distance at 700, 800 and 900 nN. The increase was not linear; rather, it exhibited sudden jumps. For instance, at 900 nN, there was a sudden increase in the number of breaking bonds at a sliding distance of 3.8 nm. This was associated with the damage mode of graphene with the AIREBO potential during the wear process. Additionally, the higher loads resulted in a greater number of breaking bonds, indicating that the load significantly impacted the wear behavior of the graphene. For REBO, LCBOP, and Tersoff, the wear-related breaking bonds in the graphene layer followed a similar pattern to that described by AIREBO, as shown in Figure 9b–d. However, the wear behavior of graphene described by REBO was more sensitive to the load compared to the other potentials, whereas Tersoff was the least sensitive, showing minimal differences in the number of breaking bonds under different loads.

The insets in Figure 9 show the sliding distance at which bond-breaking first occurred under each load. At 700 nN, the first bond-breaking in the graphene with AIREBO occurred at a sliding distance of 0.5 nm, longer than 0.3 nm (LCBOP, Tersoff) and 0.4 nm (REBO). Under different loads, the first bond breakage occurred latest using AIREBO and the earliest using LCBOP. This is consistent with the finding that the graphene with AIREBO had the best wear resistance, while the graphene with LCBOP had the worst.
The observed wrinkle formation at various angles is a result of the complex interplay between interaction force, surface roughness, and bond-breaking. Each of these factors contributes to the final deformation pattern, leading to the appearance of wrinkles at specific orientations relative to the tip.
Figure 10. Wear morphology of graphene using four potentials: (a) Tersoff; (b) REBO; (c) AIREBO; (d) LCBOP. The two long yellow dashed lines indicate the start and end of the tip. The purple dashed circle and the short yellow dashed line indicate the tip position where the graphene started to wear and the corresponding sliding distance, respectively. The solid pink circles indicate the position of the tip at the end of sliding. The pink arrows indicate the small damages. The atoms were colored according to their Z-direction heights.

Compared to the elastic deformation phase, Figure 10 also shows the larger wrinkles observed in the wear phase of graphene, primarily due to shear-induced damages and crack formations. These structural disruptions released tensile stress in the graphene and promoted compress-induced deformation of graphene; thereby facilitating the development of the wrinkles. These wrinkles greatly influenced the friction force and the corresponding coefficient of friction [38]. For the REBO potential, as shown in Figure 11a, the friction force of 26.0 nN at 700 nN in the wear phase is four times larger than 2.2 nN at 400 nN in the elastic deformation phase. At 900 nN, the friction force increased to 66.7 nN, as the wrinkles induced a large friction resistance. Damages and cracks also influenced the direct interactions between the graphene and the tip. For the four potentials, in general, the friction force increased with the load in the wear phase, which is consistent with the results in the elastic deformation phase. Due to the formation of wrinkles, however, the friction force under the same load in the wear phase no longer follows the order observed in the elastic deformation phase (e.g., Tersoff < REBO < AIREBO < LCBOP). In the wear phase, the friction force of AIREBO and Tersoff was lower than that of LCBOP and REBO. Their corresponding coefficients of friction followed a similar trend, as shown in Figure 11b. For the LCBOP potential, it should be noted that the coefficient of friction at 800 nN was close to that at 900 nN since the increase in the friction force was slower than that in the normal force [43].
Overall, within the wear phase, the order of critical load for graphene described by the four potentials is LCBOP < Tersoff = REBO < AIREBO. This result is primarily related to the distribution of the long bond. Due to the best healing ability of C–C bonds, the graphene with Tersoff has the fewest breaking bonds during the tip scratching. Due to the formation of large wrinkles and damages, the order of friction coefficients at this phase is different from that in the elastic deformation phase. The friction coefficients of AIREBO and Tersoff are lower than those of LCBOP and REBO. It is worth mentioning that in terms of computational efficiency, the time required for AIREBO to compute 1000 steps is approximately twice that of Tersoff and LCBOP, and about 1.6 times that of REBO. Thus, AIREBO has the lowest computational efficiency.

4. Conclusions

Using MD simulations, monolayer graphene was scratched with an amorphous carbon tip employing the Tersoff, REBO, AIREBO, and LCBOP potentials. By comparatively investigating the effects of these different empirical potentials on graphene’s friction and wear, it can be concluded that:

(1) The frictional process of graphene using the REBO, AIREBO, and LCBOP potentials could be divided into three distinct phases: elastic deformation, plastic deformation, and wear. However, for graphene using the Tersoff potential, the process only included the elastic deformation phase and the wear phase.

(2) The order of friction coefficients for graphene described by the four potentials under the same load was Tersoff < REBO < AIREBO < LCBOP in the elastic deformation phase. Compared to the experimental friction coefficient, the coefficients from the REBO, AIREBO, and LCBOP potentials were relatively close, while the Tersoff potential predicted a significantly lower value.

(3) The plastic deformation of graphene observed in previous experiments could be achieved using the REBO, LCBOP, and AIREBO potentials, accompanied by the formation of SW defects due to shear-induced bond rearrangement.

(4) Graphene with AIREBO demonstrated superior wear resistance, whereas graphene with LCBOP was the most susceptible to wear. Wear resistance was primarily related to the distribution of long bonds. The observed wear morphology of graphene with AIREBO and LCBOP matched previous experimental results more closely than those with REBO and Tersoff. Overall, compared to the other three potentials, AIREBO provided a description of graphene that is closest to previous experimental results.

These findings may deepen the understanding of the friction and wear behavior of graphene at the atomic scale and assist in selecting an appropriate empirical potential for more accurate simulations and better material design.

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