Full Length Article

Unraveling the friction response from selective hydrogenation of textured amorphous carbon surface

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ABSTRACT

Ultra-low friction of amorphous carbon (a-C) film can be achieved by binding to hydrogen atoms or texturing conformations. However, it remains unclear how selective surface hydrogenation affects the friction behavior of textured a-C film. In particular, the corresponding transformation of interfacial structure and the movement of hydrogen atoms have not yet been reported because of the limitation of in-situ experimental characterization. Here, textured a-C films with selective hydrogenated surfaces were prepared, and the corresponding friction response and the transformation of interfacial structure were investigated systematically using reactive molecular dynamics simulation. Results showed that introducing hydrogen atoms to the selective bump sites of textured a-C surfaces significantly reduced the friction coefficient; however, its efficiency was closely sensitive to the hydrogen content, which was related to the interfacial passivation and the repulsion effect induced by H atoms. Most importantly, the separation of –CH clusters from textured a-C surface during sliding process and their re-bonding with the naked mating a-C surface played a key role in further enhancing the repulsive effect between contacted a-C surfaces, thereby improving the anti-friction behavior, which has not been mentioned in previous studies. These results suggest a new approach to develop the high-efficient a-C friction system for applications.

1. Introduction

In recent years, the storage density of hard-disk drives has been rapidly increasing. However, to increase the storage density is to reduce the distance between the magnetic head and disk (~3.5 nm) [1,2]. Thus, wear on the magnetic pole tips is a major problem that weakens the recording performance[3,4]. In addition, oil-free lubrication is required because of the limitations of the read-write environment. Therefore, the development of nanoscale lubricating materials and technologies is urgent.

An amorphous carbon (a-C) film is a generic term for a large class of amorphous carbon-based materials, mainly composed of sp^3 (diamond phase) and sp^2 (graphite phase) hybridized networks. It exhibits excellent properties, such as high hardness, low friction coefficient, good resistance to wear and corrosion, and biocompatibility [3]. In particular, ultrathin a-C films have atomic-level smooth surfaces, making them important candidates as protective film for hard disks and related micro-electromechanical systems (MEMS) and nano-electromechanical systems (NEMS) [5,6].

In order to further enhance the anti-friction performance of a-C film, many approaches have been conducted. Among them, texturing the a-C surface has been proven to be effective for reducing friction and wear [7]. For example, Arslan et al. [8] found that a surface texture with the optimal size of the structure (100 μm in diameter and 6 μm in depth) could drastically degraded the friction and wear of a-C films by storing abrasive chips. Although a suitable surface texture achieves a synergistic improvement in anti-friction by storing graphitized abrasive chips and lubricants during sliding [9,10], it is still vulnerable to risk of reconfiguration under high pressure and heavy loads. This cannot satisfy the required overall performance of a-C films for practical applications [11,12].

In addition, the introduction of hydrogen atoms onto a-C surface is
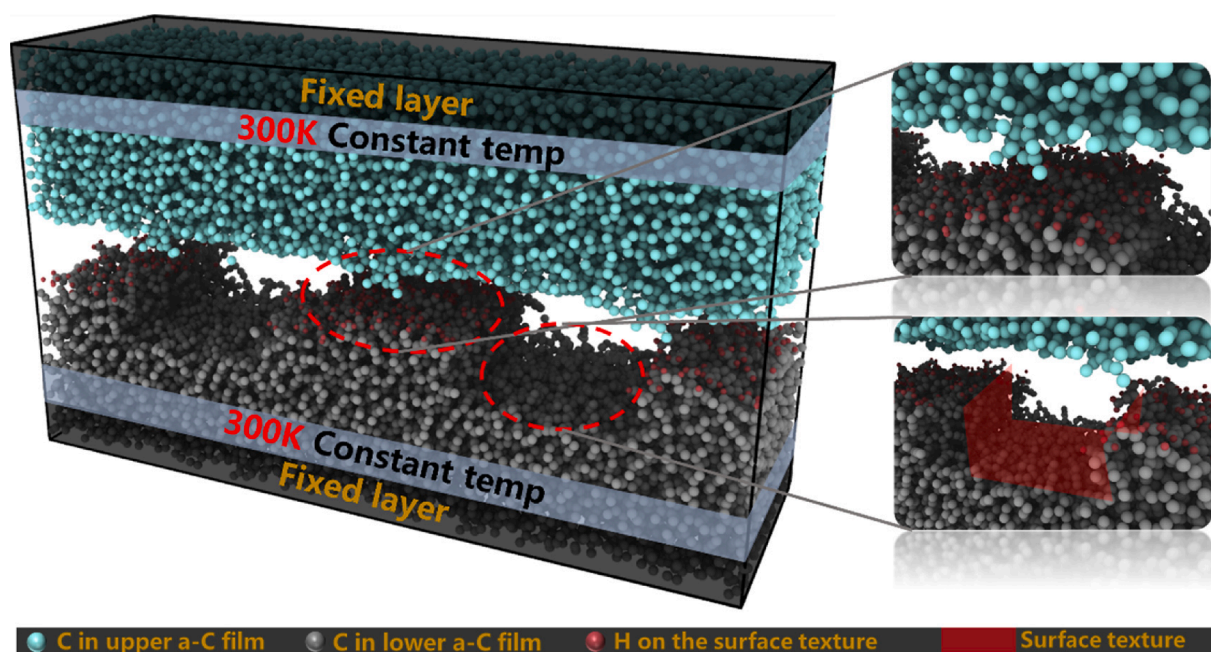

Fig. 1. Friction model consisting of textured a-C as the lower film obtained through selective surface hydrogenation and untextured a-C as the upper mating film.

also suggested, which can exhibit a super-lubricated state under vacuum and nitrogen atmospheres by passivating the unsaturated carbon atoms of the a-C surface [13,14]. For example, Erdemir et al. [15] highlighted the importance of the H/C ratio on the tribological performance of hydrogenated a-C (a-C:H) films, stating that a high H/C ratio was fundamental to achieving superlubricated properties. Wang et al. [16] combined experimental phenomena and molecular dynamics (MD) simulations to investigate the potential connection between the triboemission of hydrocarbon molecules during the friction process and tribological properties of a-C:H films.

Until now, there are few studies on the synergetic effect of both surface hydrogenation and texturing of a-C films. Song et al. [17] prepared textured a-C:H films with different groove distances and found that the most extended wear life was exhibited at a distance of 0.5 mm. It was proposed that the texture could inhibit and further trap hard abrasive debris during the friction process, thereby effectively preventing the lubrication failure of a-C:H. However, the complete hydrogenation of a-C films normally deteriorates the intrinsic mechanical properties; only surface hydrogenation, especially selective hydrogenation at the frictional contact sites of textured a-C surfaces, has never been studied. Moreover, owing to the complexity and diversity of friction interfaces and even possible interfacial reconfigurations as well as the limited in-situ experimental characterization, an accurate understanding of friction interface from macroscopic experiments remains unavailable, which causes an unclear friction mechanism and also seriously hinders the effective applications of a-C films [18–20].

In this work, considering the shielding effect of hydrogen atoms which can occupy the active sites of a-C surfaces [15,21–23] and thus prevent frictional failure of the surface texture, a textured a-C film was pre-fabricated first and then hydrogen atoms were selectively introduced onto the textured a-C surface, that is the frictional contact site of the mating a-C films, to study the coupling effect of surface texture and hydrogen passivation. The friction dependence of the textured a-C surfaces on surface hydrogen content was mainly investigated through reactive MD (RMD) simulation. In particular, the corresponding transformation of the interfacial structure, including the hybridized structure, interaction between a-C and hydrogen atoms, and the flow behavior of hydrogen atoms, were systematically explored to reveal the underlying mechanism. These results can provide theoretical guidelines

for the effective design and modulation of a-C film used as surface protective material of hard disk and MEMS components.

2. Methods

All RMD calculations were performed using a large-scale atomic or molecular massively parallel simulator [24]. Fig. 1 shows a friction model consisting of a textured a-C with selective surface hydrogenation as the lower film and an untextured a-C as the upper mating film. A three-step method was used to fabricate this model. First, the initial H-free a-C structure containing 38,875 carbon atoms was deposited using the atom-by-atom method [25], which had a size of $128.64 \times 40.36 \times 94.16$ Å^3 and an sp^3 fraction of 21 at% and sp^2 fraction of 63 at%. The initial structure was treated as an upper mating film, as shown in Fig. 1. Then, high-pressure gases with different numbers of H$_2$ molecules were introduced onto the surface of this initial a-C structure followed by annealing at 600 K to obtain hydrogenated surfaces with different hydrogen contents, as described in a previous study [26]. These hydrogenated a-C films were tailored to obtain textured surfaces with a similar rectangular shape, in which the textured width along the $\times$ direction was 30 Å, the depth along the z direction was 10 Å, and the length along the y direction was maintained at 40.36 Å. However, the hydrogen atoms at the bump location of the hydrogenated a-C surface remained (Fig. 1), resulting in the formation of selective hydrogenated textured a-C surfaces with different surface hydrogen contents, which was selected as the lower film in Fig. 1, respectively. Based on the different contents of hydrogen atoms at the surface of the lower film, the textured a-C films were named DRY@0%, DRY@10.5%, DRY@24.2%, and DRY@32.1%, respectively. Even if the texture size was smaller than that used in the experiment, it was sufficient to extract information about the in-situ friction interface and reveal the fundamental differences induced by different hydrogen contents at the textured a-C surfaces, providing insights on the designs of a-C films, particularly the nanoscale for hard disk, MEMS, and NEMS applications.

Prior to the sliding process, the friction system was divided into three layers, including a fixed layer, a thermostatic layer, and a free layer, as shown in Fig. 1. The fixed layer was used to simulate an infinite system. The thermostatic layer was a constant temperature layer consisting of an NVE set of a Berendsen thermostat maintained at 300 K [27]. The free
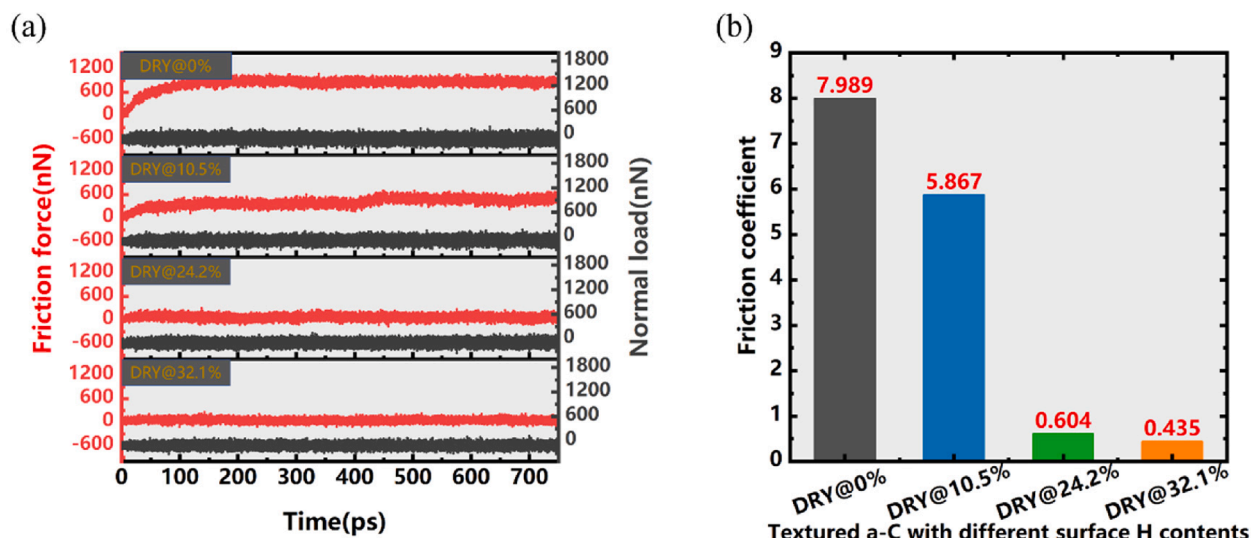
Fig. 2. Friction properties of the different systems: (a) friction force and normal load curves of each system with sliding time and (b) dependence of friction coefficient on the surface H contents of lower textured a-C film.

layer comprised the remaining a-C and hydrogen atoms, which were used to simulate the friction-induced structural evolution at the interface. The time step was 0.25 fs and periodic boundary conditions were imposed in both the × and y directions. The ReaxFF potential developed by Tavazza et al. was used to describe the C–C, C–H, and H-H interactions in the entire system [28], and its reliability and accuracy were validated in our previous studies [12,25,29,30].

During the friction simulation, the entire system was first relaxed at 300 K within 2.5 ps, and then the upper a-C film was loaded onto the lower textured a-C film within 25 ps until the specified contact pressure value was reached. Finally, the fixed layer of the upper a-C film was applied with a constant sliding speed (100 m/s) along the x direction for 750 ps. It should be noted that a contact pressure of 5 GPa has been

found suitable for studying the friction behavior of a-C films at the atomic scale [31–34]. Furthermore, due to simulation time and computing resource constraints, a higher sliding velocity is required to simulate a longer sliding distance and sample sufficient spatial phases [12,29].

3. Results and discussion

To evaluate the effects of the degree of surface hydrogenation on the frictional characteristics of a-C films, the friction and normal load values for each time step are calculated from the total number of fixed atoms operating in the bottom a-C layer along the sliding direction, as shown in Fig. 2(a), which shows the friction and normal load curves with respect
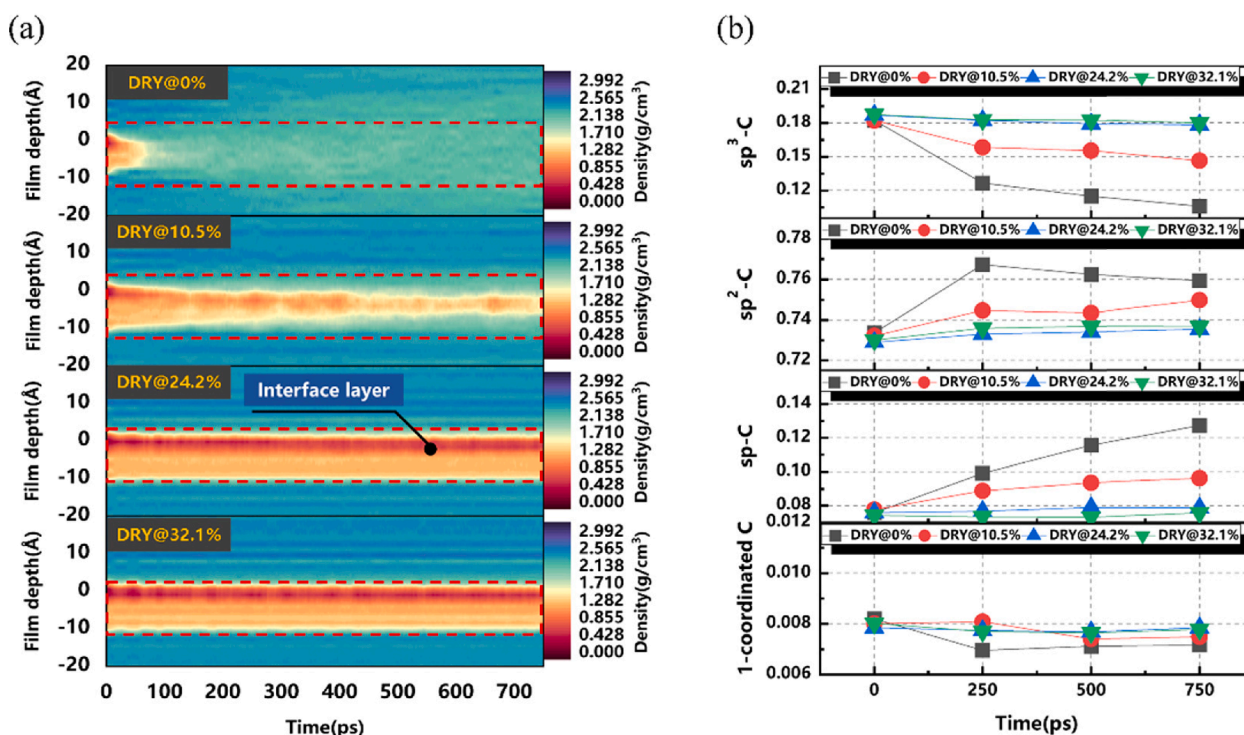

Fig. 3. Structural evolution of system: (a) density distribution and (b) changes in the fractions of sp³-C, sp²-C, sp-C, and 1-coordinated C hybridized bonds.
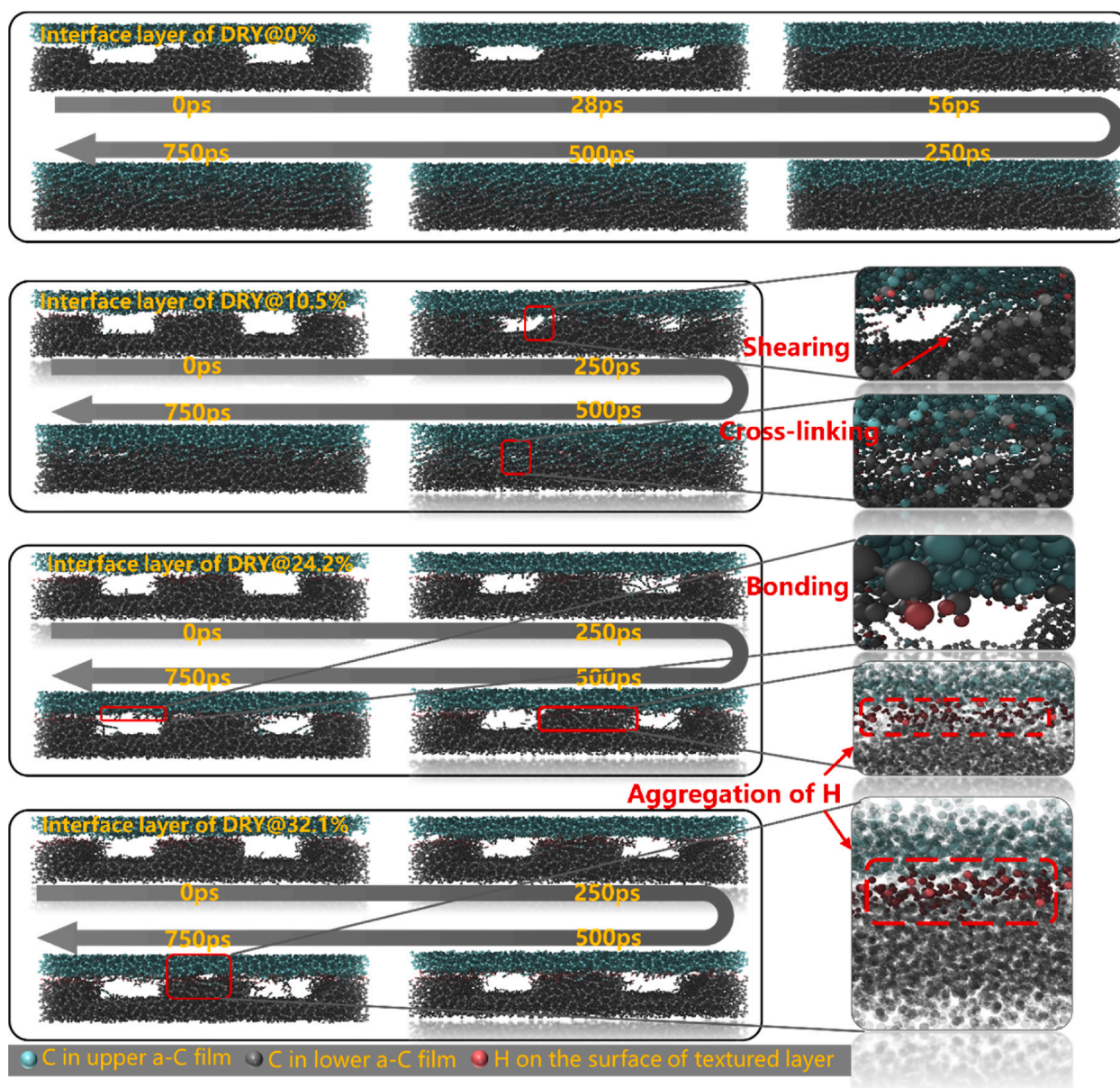
Fig. 4. Evolutions of interfacial morphologies of friction systems with different surface H contents of the lower textured a-C films during the sliding process.

to frictional sliding time [30]. The results indicate that for each system, the friction force initially increases with sliding time and then remains steady until the sliding is completed. However, the friction curves exhibit a substantial correlation with the hydrogen contents of the textured a-C surfaces. The DRY@0% system shows a high friction force and significant running-in process. In contrast, the friction force is reduced considerably, and the running-in process is also shortened with an increase in the surface hydrogen content. The friction curves of the DRY@32.1% system are similar to those observed in oil lubrication, suggesting that hydrogen atoms may act as barriers to prevent a-C surfaces from coming into contact with each other [30].

The average friction force and normal load during the steady-state friction stage are calculated using the values of the last 200 ps to quantify the effect of different surface hydrogen contents on friction behavior. As shown in Fig. S1 of Supporting Information, the results show that system with higher hydrogen content has reduced friction, demonstrating the critical function of hydrogen atoms in friction reduction [14]. The friction coefficient is estimated using the average friction force and normal load values. Fig. 2(b) shows that the friction

coefficient decreases monotonically with increasing hydrogen content. Compared to the DRY@0% system, DRY@32.1% results in a 95% reduction in the friction coefficient, which exhibits the best anti-friction ability compared to DRY@10.5% and DRY@24.2%. In addition, the values for the friction coefficient obtained from the present simulations are generally higher than the experimental values, as shown in Fig. 2(b), which is attributed to the high bonding strength of the mating materials caused by the absence of surface pollution and passivation [12,25].

To explore the potential friction mechanism induced by the different surface hydrogen contents of lower textured a-C, the transformation of the interfacial structure, which is closely related to friction behaviors, has to be analyzed [26]. First, it is necessary to explore the changes in the physical properties of the interface. As shown in Fig. 3(a), the density of the system tends to be stabilized with the increase of surface hydrogen content. For DRY@0% system, the drastic change in density implies the collapse of the structure. For DRY@10.5% system, the introduction of hydrogen atoms effectively improves the physical structure of the interface. However, for the highly hydrogenated system, such as DRY@24.2% and DRY@32.1%, the interface layer remains stable even
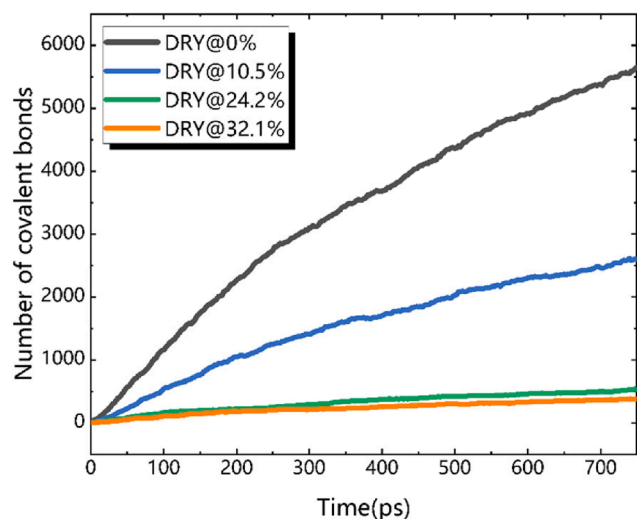
Fig. 5. Change in the number of covalent bonds between mating a-C surfaces caused by cross-linking during the sliding process for each case.

at the end of sliding process, suggesting that the change of hybridized structure mainly occurs at the interface layer.

Considering the drastic change of the mass density in the system, especially DRY@0%, the hybridized structure is analyzed based on the whole system rather than just the interface layer. Fig. 3b shows the changes in the hybridized structure during sliding process. The results of the DRY@0% and DRY@10.5% systems show that with sliding time ranged from 0 to 750 ps, the sp^3 fraction decreases, whereas the sp^2 and sp fractions increase. As a result of shearing effects, the sp^3 structure is converted into an sp^2 structure, which is thermodynamically more stable. In addition, re-hybridization of the mating surface leads to a dramatic change in the interfacial structure during sliding process. However, the sp^3 structure increases with increasing hydrogen content, which indicates an improvement in the interfacial passivation. For DRY@24.2% and DRY@32.1% systems, the a-C hybridized structures almost have no charge during the sliding process, indicating that hydrogen-induced passivation makes the a-C surface chemically stable. Changes in the hybridized structures induced by different hydrogen contents indicate the dominant role of hydrogen atoms in anti-friction properties.

The introduction of hydrogen atoms passivates the unsaturated carbon atoms at the a-C surface, which makes the interfacial structure more stable, explaining to some extent the reduction in the friction coefficient [14,35]. However, the mechanism by which hydrogen-induced passivation improves the sliding interface during the sliding process remains unclear.

Fig. 4 shows the evolutions of interfacial morphologies of friction systems with different surface H contents of the lower textured a-C films during the sliding process. In the DRY@0% system, the textured layer is deformed due to shearing at approximately 28 ps and completely collapsed at approximately 56 ps. In contrast, the collapse of the textured layer is also observed in the DRY@10.5% system. However, the duration of the collapse is significantly prolonged, suggesting that the presence of hydrogen atoms prevents the cross-linking and re-hybridization of the mating a-C. However, its efficiency strongly depends on the content of hydrogen atoms. A clear frictional contact interface is still observed at the end of the sliding process in system with high hydrogen content, indicating that the system with high hydrogen content further passivates the a-C interface by shielding the C–C covalent bonding, as confirmed by the above-mentioned analysis of hybridized structure (Fig. 3).

In addition, in system with high hydrogen content, the aggregation of the hydrogen atoms at the interface forms a hydrogen-rich layer (Fig. 4). A similar phenomenon was observed by Li [25]. This causes a regional concentration of atomic hydrogen stress. Although the breaking of C–H bonds is not observed, Fig. 4 clearly shows a large number of –CH clusters separated from the lower textured a-C and re-bonded to the upper naked a-C surface. This is contrary to those reported by Erdemir and Kubo [36,37].

Moreover, as indicated in Fig. S2 of Supporting Information, a small number of larger hydrocarbon molecules are found at the interface. A similar phenomenon is observed in Wang's study [16]. Interestingly, at the end of the sliding process, the a-C bond angles at the upper surface tend to be parallel to the sliding direction. Such an ordered surface structure also contributes to the decrease in the friction coefficient [38]. The potential connection between these phenomena and the reduction in the friction coefficient is explored in detail below.

Prior to that, the change in the number of C–C covalent bonds between the mating a-C surfaces caused by cross-linking is recorded for each system during the sliding process. The final bonding at each time step is counted without the process from breaking to bonding [16]. As shown in Fig. 5, the number of bonds in DRY@0% and DRY@10.5%
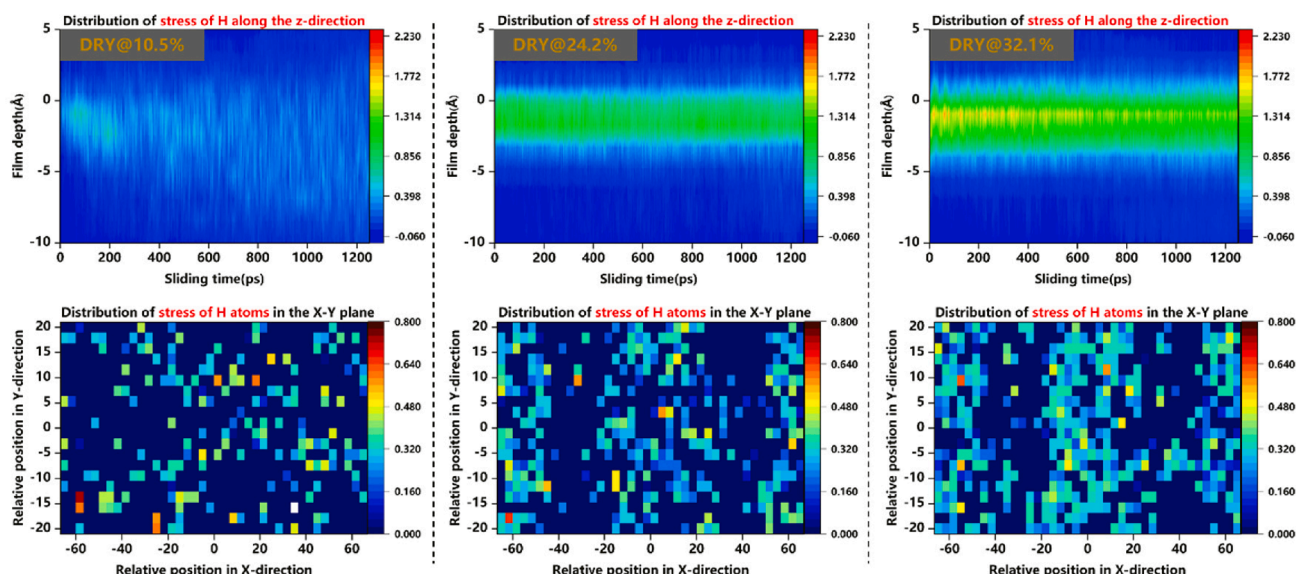

Fig. 6. Stress distributions of hydrogen atoms in the various systems with sliding time and their heat maps in the X-Y plane at the end of the sliding process.
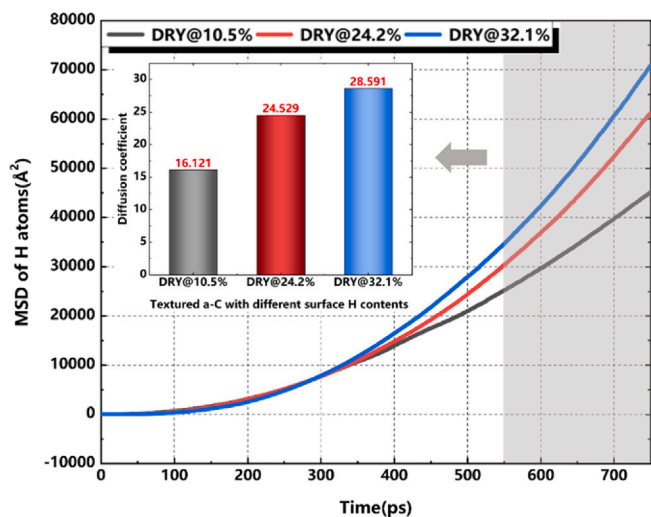
Fig. 7. MSD curve and diffusion coefficient of H atoms along the sliding direction for each system.

systems increase quickly with sliding time. In contrast, the presence of a large number of hydrogen atoms in DRY@24.2% and DRY@32.1% systems almost isolate the C–C bonding, which provides quantitative evidence for the passivating effect of hydrogen atoms on the friction interface.

As shown in Fig. 6, the hydrogen atoms exhibit tensile stress during the sliding process, which corresponds to strong repulsive force. In systems with higher hydrogen contents, the hydrogen atom stress is mainly distributed at the sliding interface, which corresponds to the aggregation of hydrogen atoms, as shown in Fig. 4. The corresponding stress concentration is more pronounced in the DRY@32.1% system. Furthermore, at the end of the sliding process, the heat maps in the X-Y plane for the stress distributions of the hydrogen atoms are provided. The results show that hydrogen atoms are mainly present on the textured bump surfaces. The hydrogen atoms also tend to concentrate regionally as the hydrogen content increases, resulting in a reduced contact area, which supports the reduction in the friction coefficient. In the DRY@10.5% system, many hydrogen atoms are subjected to relatively large forces due to cross-linking and re-hybridization, where repulsive interactions between hydrogen atoms are hindered and interactions with intrinsic a-C are enhanced. For the DRY@24.2% and DRY@32.1% systems, strong repulsive interaction between hydrogen atoms separates the upper and lower a-C surfaces, as shown in Fig. 4.

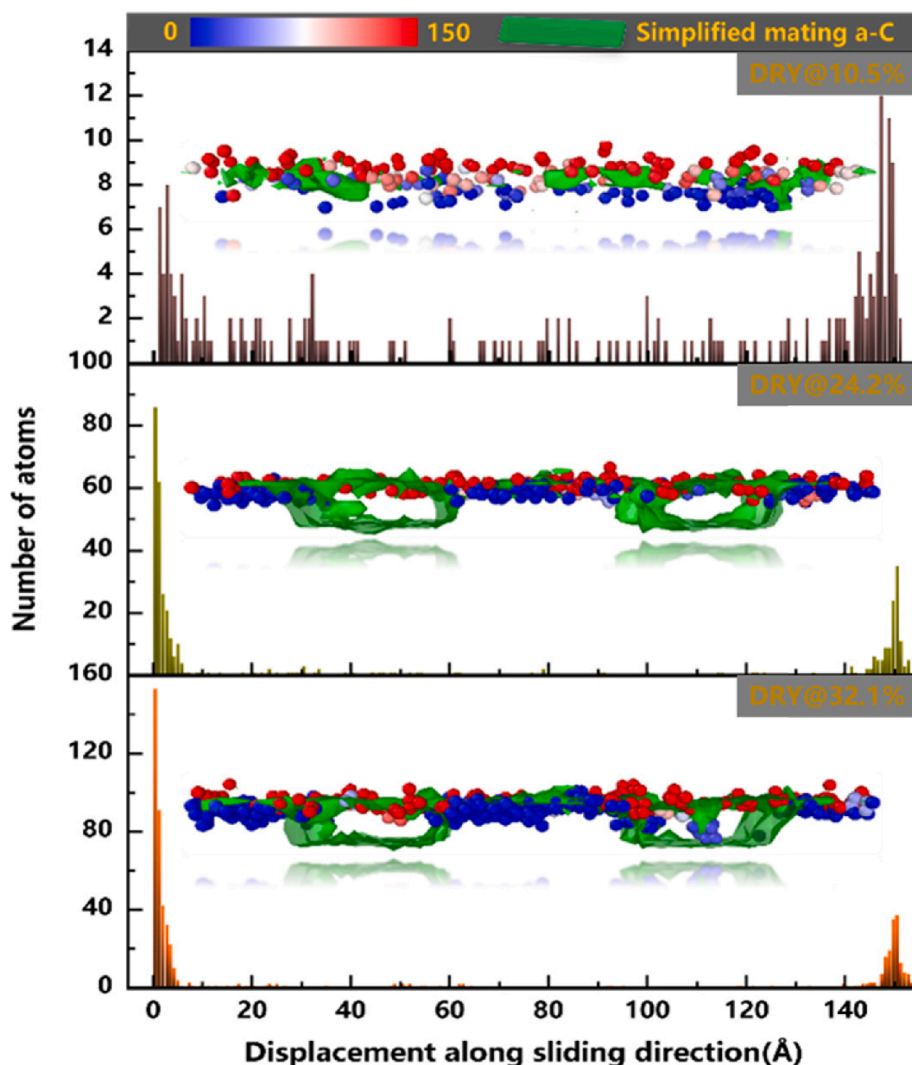The behavior of the hydrocarbon molecules bonded to the surface of

Fig. 8. Displacement of hydrogen atoms in the last 150 ps during the sliding process for each case.
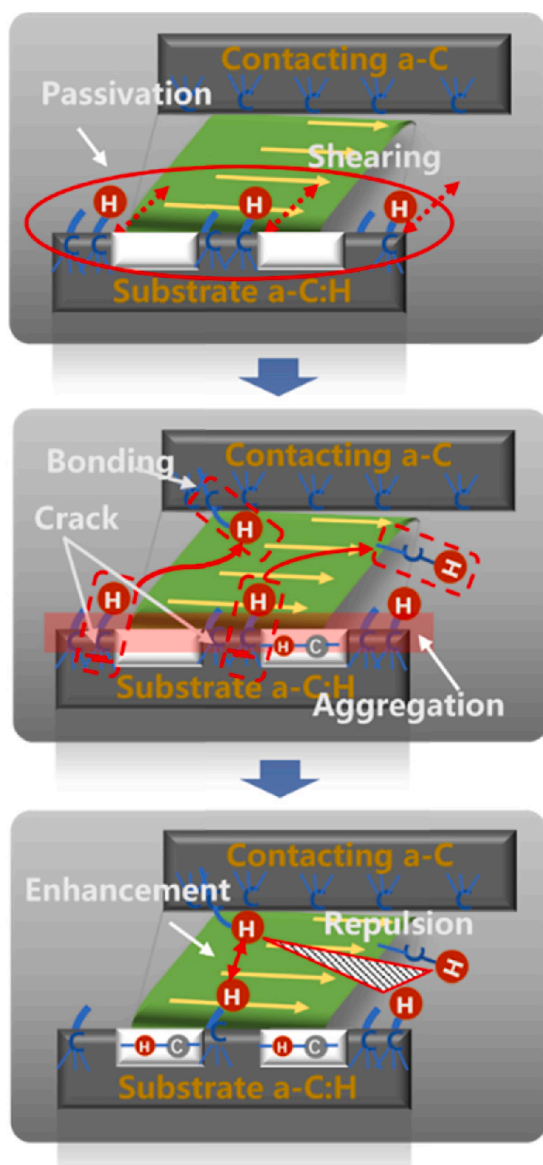
Fig. 9. Friction mechanism of textured a-C film caused by selective surface hydrogenation.

upper a-C in Fig. 4 indicates the possible mobility of the hydrogen atoms. To describe the mobility of hydrogen atoms in the various systems, the mean square displacement (MSD) of the hydrogen atoms during sliding is plotted. As shown in Fig. 7, the MSD increases gradually with the sliding time and strongly depends on the hydrogen content. Based on the MSD values marked with gray backgrounds, the diffusion coefficient of the hydrogen atoms along the sliding direction is calculated for each case, which increases monotonously as a function of hydrogen content.

The MSD curves show an unexpectedly high mobility, implying that some hydrogen atoms follow the flow of upper a-C. This is the main effect of repulsive forces between hydrogen atoms on friction reduction. First, the number of hydrocarbon bonds during the sliding process are calculated to determine the behavior of the flow of the hydrogen atoms. As shown in Fig. S3 of Supporting Information, the number of hydrocarbon bonds barely changes during sliding process, indicating that the C–H bonds are not broken. Combined with the C–C bonding shown in Fig. 4, it is qualitatively demonstrated that the friction-induced shearing effect breaks the C–C bond, not the C–H bond. Most of the broken hydrocarbon clusters carrying hydrogen atoms are re-bonded to the carbon atoms at the naked upper a-C surface and thus follow their flow

behavior.

Fig. 8 shows the displacement of hydrogen atoms in the last 150 ps of the sliding process, in which the different colored particles indicate the magnitude of the displacement. It can be observed that the majority of hydrogen atoms show low and high mobilities. The atoms with low mobility are those that are stable on the lower bump surface; the high mobility of atoms is caused by their bonding with the upper sliding surface. However, there are also some hydrogen atoms exhibiting tiny displacements in the form of free hydrocarbon molecules at the friction interface, as presented in the Fig. S2 of Supporting Information. DRY@10.5% system exhibits anomalous mobility of hydrogen atoms owing to cross-linking of mating a-C films. For DRY@24.2% and DRY@32.1% systems, despite the relatively small number of hydrogen atoms with high mobility, they contribute most of the MSD in the sliding process. Most importantly, these highly mobile atoms bonded with the upper surface provide a more stable repulsion with those on the lower surface during the sliding process, resulting in an easy shearing of the friction interface [32]. This not only enhances the mobility of the hydrogen atoms but also causes a further reduction in friction, thus resulting in low friction coefficients, as illustrated in Fig. 2.

The improvement in the friction properties of the textured a-C films caused by selective surface hydrogenation is demonstrated. It shows the effect of hydrogenated textured surface on the friction properties of a-C film. As shown in Fig. 9, the main mechanisms are as follows.

- The addition of hydrogen atoms onto the bump surface of the lower-textured a-C film shows a significant passivating effect on the active a-C surface. At low hydrogen contents, the exposed a-C surface suffers structured depressions and is vulnerable to hybridization. With increasing hydrogen content, sufficient hydrogen atoms prevent a-C from coming into contact with each other, drastically reducing the friction.
- During the sliding process, on the one hand, the hydrogen atoms tend to be stabilized on the surface of the structured bump, resulting in a large number of hydrogen atoms clustering regionally and generating high tensile stresses. On the other hand, the shearing effect breaks the C–C bonds on the lower surface rather than the C–H bonds, generating many –CH clusters. Most of these separated hydrocarbon clusters re-bond to the upper mating a-C surface, whereas a small number are free at the friction interface.
- The hydrogen atoms bound to the upper a-C surface produce a stable repulsive effect with the hydrogen atoms on the lower surface. The enhanced repulsive effect facilitates the sliding of the friction interface, further reducing the friction coefficient of the system. In conjunction with Wang's report [16], frictional emission phenomena under regular textural condition indicate that abrasive chip storage is observed from the atomic-level.

4. Conclusion

In this study, the friction properties of textured a-C films with selective surface hydrogenation and associated tribochemical reactions were investigated using RMD simulations to determine the underlying friction mechanism. The results contributed to the following conclusions:

1) The introduction of hydrogen atoms significantly reduced the friction of the textured a-C film, and the friction coefficient monotonically decreased with increasing surface hydrogen content.
2) The strong connection between mating a-C surfaces created by C–C cross-linking and bonding prevented the friction interface from sliding, resulting in a high friction coefficient for the DRY@0% system.
3) For the DRY@10.5% system, the introduction of hydrogen atoms passivated the friction interface and reduced the degree of cross-linking between mating a-C surfaces. With a further increase in the

surface hydrogen content, such as DRY@24.2% and DRY@32.1%, the friction interface was highly passivated to shield the contact between the mating a-C surfaces. In addition, a large aggregation of hydrogen atoms occurred at the friction interface during sliding, generating a high tensile stress. In particular, the separated –CH clusters from the lower textured surface re-bonded with the naked upper a-C surface, enhancing the repulsive effect between the hydrogen atoms. These factors contributed to the drastic decrease in the friction coefficient. However, the structural ordering of the upper a-C along the sliding direction observed in this study also had a favorable effect on the anti-friction property.

4) This study demonstrated the effect of the selective hydrogenation degree of textured a-C surface on friction behavior and elucidated the fundamental mechanism. These results can provide guidance and insight on the design and regulation of textured a-C with high performance for applications, particularly in the fields of hard disks and MEMS/NEMS systems.

CRediT authorship contribution statement

Naizhou Du: Conceptualization, Data curation, Formal analysis, Methodology, Investigation, Visualization, Writing – original draft. **Xubing Wei:** Formal analysis, Methodology, Investigation, Writing – original draft. **Xiaowei Li:** Conceptualization, Data curation, Funding acquisition, Investigation, Resources, Supervision, Writing – original draft, Writing – review & editing. **Zan Chen:** Formal analysis, Writing – original draft. **Shiqi Lu:** Formal analysis, Writing – original draft. **Jiaqing Ding:** Formal analysis, Writing – original draft. **Cunao Feng:** Formal analysis, Writing – original draft. **Kai Chen:** Formal analysis, Writing – original draft. **Jianghao Qiao:** Formal analysis, Writing – original draft. **Dekun Zhang:** Conceptualization, Supervision, Writing – review & editing, Resources. **Kwang-Ryeol Lee:** Conceptualization, Supervision, Writing – review & editing, Resources.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Acknowledgement

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.apsusc.2022.156246.

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