

Effect of environmental hydrogen atoms on the tribological behaviors of diamond-like carbon films



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ABSTRACT

Influence of environmental H atoms on the tribological behaviors of DLC films is investigated via molecular dynamics simulations. These H atoms significantly reduce the friction force, and the reduction mechanisms depend on friction temperatures. At low friction temperatures, the H atoms are concentrated near contact interfaces, and their passivations highly reduce the interfacial adhesion, resulting in the low friction force. However, high friction temperatures induce the significant diffusion of the H atoms into the DLC films and thermally expand such films and increase their graphitization, causing a wide region with easy-shear properties to reduce the friction force. It is believed that these mechanisms of friction reduction can improve the understanding of the superlow friction of DLC films in H₂ environment.

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1. Introduction

Diamond-like carbon (DLC) or amorphous carbon films are formed by carbon atoms via sp³, sp² and sp hybridized bonds [1]. These films exhibit high mechanical strength, good chemical inertness and excellent tribological behavior and thus have been used widely as solid lubricants.

Superlubricity (or superlow friction) is a motion regime in which adhesion or friction almost vanish [2]. This regime is urgently pursued since it can help to save the large amounts of energies consumed by friction in many moving mechanical systems. The superlubricity of the DLC films can be commonly achieved by tailoring their bulk microstructures and surface properties [3]; however, recent studies have shown that it can also be observed when the test atmosphere is hydrogen H₂ [4–9]. The atmosphere-induced superlubricity of DLC films has attracted wide attentions since its discovery [4]. Previous experimental works demonstrated that the superlow friction of these films in the H atmosphere is attributed to the passivation of surface dangling bonds by H atoms instead of H₂ molecules through tribochemical reactions [4–7]. Simulations of the relative sliding of DLC films further demonstrated that a repulsive force would increase dramatically as the H-passivated carbon surfaces get close, thus suppressing the formation of covalent bonds between them [8–10]. As a result, the interface adhesion and the sliding friction are highly reduced.

However, mechanisms of friction reduction induced by huge repulsive forces are only applicable to the running-in stage of friction but not to its stable stage. This is due to the fact that for the relative sliding of DLC films their contact surfaces can be distinguished only in the running-in stage but be mixed with each other in the stable friction stage [11]. This mixing process can break the C–H bonds at the contact surfaces and promote H atoms to diffuse into the DLC films [12]. These diffusions were observed in the latest study by Erdemir et al. [6]. Their analysis of element distributions showed that the wear track of DLC films becomes rich in H atoms in the stable friction stage.

Investigations of the H-atom diffusions and their influences on the friction reductions of DLC films have been rarely reported. In the present study, the issue of H-atom diffusions is studied by molecular dynamics (MD) simulations. By adding H atoms instead of H₂ molecules at the contact interface of DLC films, their relative sliding after the complicated tribochemical reactions from H₂ molecules to H atoms in experiment can be directly simulated. The interface evolution as well as the diffusions of H atoms can be observed in the simulation, and the mechanisms of friction reductions are discussed in detail.

2. Modeling

As illustrated in Fig. 1, the atomistic simulation model consists of two DLC films and a random distribution of hydrogen atoms at their interface, which is located at the x–z plane of the Cartesian

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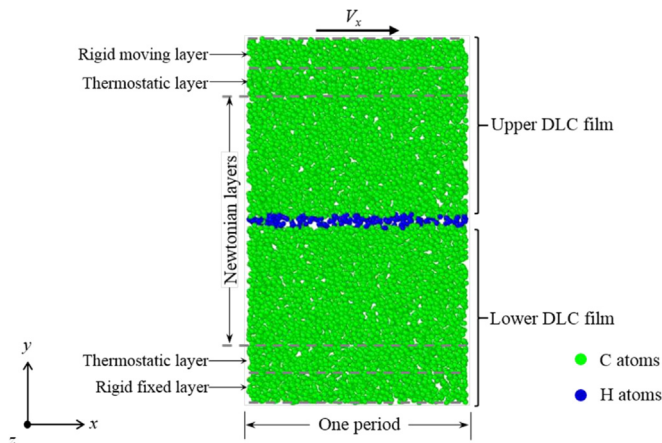


Fig. 1. Illustration of the friction model.

coordinate system x - y - z . The upper DLC film slides against its lower counterpart along the x -direction in the velocity of V_x .

The periodic boundary conditions are applied along both the x and z -directions. Along the y -direction, both the upper and lower DLC films can be divided into three layers. The upmost one of the upper film is defined as a rigid body to keep its structure undeformed. The velocity V_x is applied to this rigid layer to realize the sliding of the whole upper film, and the load F_n is also applied to it along the y -direction. The lowest one of the lower film is also defined as a rigid body but its location is fixed. The other layers contain the Newtonian atoms which can move freely under the forces of neighbors according to Newton's second law of motion. The layers adjacent to each rigid one in the both films are coupled to a thermostat which keeps a constant temperature at 300 K by rescaling velocities of atoms. This thermostat can dissipate the friction heat that is generated at the sliding interface. The rest layers are the Newtonian ones. Particularly, the H atoms are also Newtonian atoms and contained into a Newtonian layer. More details can refer to our previous study [13].

Both the upper and lower DLC films are obtained by a same melting-quenching procedure [14]. In this procedure, a crystalline diamond film comprised of 4544 atoms is initially generated with periodic boundary conditions along all the x , y and z -directions in a canonical NVT ensemble at 300 K. The temperature of the system is then increased to be above the melting point of diamond. Afterwards, the system is thermostatically equilibrated for about 20 ps and then cooled down to 300 K at a rate of 1000 K/ps which allows proper relaxation of the amorphous structure [15]. The isothermal-isobaric NPT ensemble is finally employed to eliminate the residual stress in the film by relaxing its structure at 300 K. All the adjustments of temperatures are controlled by the Nose-Hoover method. The final dimensions of the obtained film are 47.4 Å, 38.5 Å, and 15.8 Å along the x , y and z -directions, respectively.

The simulations are conducted by the large-scale atomic/molecular massively parallel simulator (LAMMPS) [16]. The atomic interactions are described by the adaptive intermolecular reactive empirical bond order (AIREBO) potential which was developed to model both chemical reactions and intermolecular interactions in hydrocarbon systems [17]. The long-range repulsive forces in this potential are neglected because they can lead to the occurrence of gas-lubrication friction instead of solid-contact friction by highly increasing the distances between C and H atoms and thus prevent the diffusions of the H atoms into DLC films. The time step of simulations is set as 0.5 fs, and each of them lasts 250 ps. Molecular visualization is realized by the software of OVITO [18].

During the simulation, the friction force F_f is obtained by calculating the tangential force of the upper rigid layer along the x -direction. To show the microstructural evolution, the friction system is divided into multiple strips along the y -direction. In each strip, the number of H atoms, the average temperature and the fractions of sp^3 hybridized C atoms are evaluated. The fraction is defined as the ratio of the number of the sp^3 C atoms in each strip to the number of the C atoms in it. The temperature is calculated based on its relation with the kinetic energies of atoms [13]. The hybridization states of carbon atoms are defined by their coordination numbers which are obtained by calculating the number of nearest atoms within the cutoff length of 2.0 Å for C-C pairs and 1.5 Å for C-H pairs [19]. The fourfold, threefold and twofold carbon atoms are regarded as sp^3 , sp^2 and sp bonded, respectively [14].

The load is applied by adding uniform forces along the y -direction to each atom in the upper rigid layer prior to the sliding commencement. The effects of the density of H atoms D_H on friction force F_f are studied under various testing conditions. The D_H with the unit of atom number per area on the interface varies from 0, 10.6 to 27.6 nm^{-2} . Three testing conditions are considered. For the reference case, the load F_n and the sliding velocity V_x are set as 0.9 nN and 1 Å/ps, respectively. These two testing parameters increase separately in high-velocity case ($F_n=0.9$ nN and $V_x=5$ Å/ps) and in high-load case ($F_n=9$ nN and $V_x=1$ Å/ps).

3. Results and discussions

3.1. Friction force and atomic configurations

The friction force F_f with different densities of H atoms D_H in various testing cases is shown in Fig. 2. With the commencement of sliding, the F_f increases and then reaches its maximum value followed by a sharp drop. The increase is attributed to that the high adhesive force caused by the C-C covalent bonds across the interface between DLC films can induce their shear deformations during the sliding. The sharp drop corresponds to the breakings of such bonds when the films yield. Afterwards, the F_f stabilizes with stick-slip patterns and becomes larger after its stabilization. The average stabilized F_f is about 250 nN for both $F_n=0.9$ nN and $F_n=9$ nN when $V_x=1$ Å/ps and H atoms are absent. This stabilized F_f is close to those in literature [20–22], which can help to verify the validations and accuracy of present simulation model.

The presence of H atoms can significantly induce the reduction of friction force F_f both before and after its stabilization (Fig. 2a). The H atoms can also delay the stabilization of F_f . When $D_H=0$, the F_f becomes stable at the simulation time of about 40 ps. However, F_f stabilizes at 60 ps for $D_H=10.6$ nm^{-2} and at 80 ps for $D_H=27.6$ nm^{-2} .

Under a large load F_n (Fig. 2b), the F_f before its stabilization increases for $D_H=0$ and $D_H=10.6$ nm^{-2} but is almost unvaried for $D_H=27.6$ nm^{-2} . After the stabilization of F_f , the magnitude of its stick-slip patterns is slightly raised for $D_H=10.6$ nm^{-2} and $D_H=27.6$ nm^{-2} , whereas keeps constant for $D_H=0$. This slight raise indicates that the influence of the H atoms on the reduction of F_f is slightly weakened at the large F_n .

When the sliding velocity V_x increases (Fig. 2c), the F_f is highly reduced both before and after its stabilization. Such reduction may be due to the higher friction temperature induced by the higher V_x . Particularly, the F_f after its stabilization for $D_H=27.6$ nm^{-2} is only slightly smaller than those for $D_H=0$ and $D_H=10.6$ nm^{-2} . This implies that the effect of the H atoms on the reduction of F_f is highly eliminated by the high V_x .

Atomic configurations of DLC films with various densities of H atoms D_H before the stabilization of F_f are illustrated in Fig. 3. An inner straight red marker defined before the sliding is employed to

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