



Effects of atomic structure on the frictional properties of amorphous carbon coatings

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ABSTRACT

Diamond-like carbon (DLC) films are widely used as protective coatings against wear and corrosion and have attracted a lot of attention in the last few decades. However, it is very difficult to determine the hybridization and structure of amorphous carbon experimentally during sliding. Therefore, in this work, molecular dynamics (MD) simulations are employed to investigate the nano-tribological properties of amorphous carbon with and without hydrogen atoms doped. The simulation models are built with DLC/DLC interface and diamond/DLC interface for different densities of carbon. As we found, both the carbon bonding network and the carbon hybridization have significant effect on the frictional properties of DLC films. The unsaturated carbon atoms, which are in sp^2 or sp^1 hybridization, can lead to the formation of covalent bonds between the two contacting surfaces resulting in stick-slip type of friction. With an increase of sp^3 bonding content in tetrahedral carbon and doping of amorphous carbon with hydrogen atoms decrease the steady-state value of friction force and reduce the amount of the stick-slip motion.

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1. Introduction

Amorphous diamond-like carbon (DLC) films have attracted substantial attention over the past few years due to their excellent material properties, such as high hardness, low friction coefficient and high inertness [1,2]. DLC films are widely used as protective coatings against wear and corrosion in areas such as high-precision bearings, mechanical seals, micro/nano-electromechanical devices (MEMS/NEMS) and hard disk drives [3,4]. DLC films are amorphous carbon coatings which contain a mixture of sp^2 and sp^3 hybridizations. Their tribological properties depend on the ratio of sp^2 and sp^3 bond, hydrogen content and the presence of dopant atoms, e.g., Si [5]. The friction coefficient of DLC films ranges from 0.003 to 0.7, as reported in Refs [6–8] and can be affected by test conditions [9,10], e.g., distance, loading rate, counterface material [9] and environmental conditions [11,12]. Hence, it is important to study the effects of hybridization content and atomic structure on the mechanical and tribological properties of DLC films.

Mechanical and tribological properties of DLC films have been reported in numerous studies both experimentally [13–18] and numerically [19–28]. Mohrbacher et al. [15] investigated the friction mechanism of DLC films by rubbing DLC with corundum, and found that the coefficient of friction (COF) decreases with increasing normal contact force. Fontaine et al. [16] found a super low friction state with

a friction coefficient of 0.002 by performing sliding tests between DLC films and iron surfaces under high-vacuum conditions (10^{-7} Pa). Erdemir investigated the friction and wear performance of DLC films experimentally and showed that hydrogen doping plays an important role in the friction and wear performance of DLC films [17]. Sunmat et al. experimentally studied the effects of surface chemistry and hybridization state in nanostructured carbon-based materials on nano-scale mechanical, chemical, and tribological properties. They found that the adhesion and friction of ultrananocrystalline diamond are both reduced after hydrogen termination [18]. Cui et al. also experimentally found that the adhesion between mating materials and carbon can greatly affect the vacuum tribological behaviors of DLC films [19]. They declared that choosing mating materials with low adhesion to carbon to avoid formation of transfer films at the interface is a promising method for achieving low friction and long wear life of DLC films in high vacuum.

Although there have been studies on the tribological properties of amorphous carbon, details of the underlying mechanisms are not well illustrated. In addition, it is difficult to investigate the effect of all the parameters, such as loading control, loading speed, and environmental conditions, on the tribological properties of DLC. Furthermore, determining changes in the hybridization and chemical reactions of carbon atoms in a DLC film during sliding is very challenging, especially for atomically thin amorphous carbon films. Molecular dynamics (MD) is an appropriate tool to simulate the mechanical properties and friction mechanism of amorphous carbon because positions, forces and velocities of all atoms are known as a function of time [20]. Gao et al. [21]

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investigated the tribo-chemical reactions between pure diamond and DLC films during sliding and found that hydrogen can affect the surface of DLC films and thus affect the friction. Knippenberg et al. studied contact forces between a spherical tip and a self-assembled monolayer composed of C14 alkane chains and found that the monolayer atoms contributed to the change in friction [22]. Pastewka et al. investigated the running-in of two hydrogen doped amorphous carbon films using molecular dynamics [23]. A further step into the direction of realistic sliding friction simulations was made by Pastewka et al. [24] in order to study the run-in, lubrication, and failure of hydrogenated DLC coatings on an atomic scale. Molecular dynamics simulations were also employed by Schall et al. [5] and Hayashi et al. [25] to study the effect of film structure, passivation, adhesion, tribochemistry, and contact load on the tribological behavior of self-mated DLC contacts. Bai et al. [26] investigated friction reduction in DLC films by using MD and quantum chemical method and found that the presence of hydrogen and fluorine atoms can lead to ultra-low friction. The tribological properties of DLC films are affected by various factors, such as the amount of sp^3 bonding, the amount of hydrogenation and the presence of dopant atoms. However, the MD studies mentioned above only focus on systems in which the surfaces are saturated with hydrogen or other materials, and no chemical reaction or single hydrogen abstraction events are simulated.

There are limited MD studies in the literature that deal with the rehybridization mechanism of tetrahedral amorphous carbon (ta-C) and diamond coatings during sliding [27–29]. Gao et al. [27] conducted a MD study of hydrogen-terminated diamond (111) in sliding contact with amorphous, hydrogen-free carbon films in order to investigate the effect of film thickness and adhesion on the tribological properties of DLC films. It was shown that tribochemical reactions can lead to adhesion between the counterface and film [27]. Kunze et al. [28] proposed that the wear occurring on ta-C/ta-C and diamond/diamond surfaces is dictated by presence of the amorphous sp^2 (a-C) interlayer formed at the interface due to the rehybridization of sp^3 and sp^2 bonds. According to Kunze et al., rehybridization is mainly caused by a tribomechanical rather than a tribothermal process. Graphitization was observed at the interface when the interface temperature was well below the material melting temperatures. Continuous changes in the atomic force network at the ta-C/a-C interface during sliding affect the structural integrity of the deeper layers in ta-C and promote rehybridization [28,29].

As can be seen from the above literature review, most of the experimental [13–19] and numerical [20–29] work has been done on studying the mechanical and tribological properties of hydrogen-terminated DLC films. No work that studies change in the carbon bonding network during sliding of hydrogen free amorphous carbon has been found in literature. In addition, studies of the effect of sp^3/sp^2 ratio on the tribological behavior of hydrogen free amorphous carbon are still missing. For low-friction of DLC films, there are two essential lubrication mechanisms described in literature: chemical passivation of dangling bonds of carbon atoms at the sliding interface, known as ‘passivation mechanism’ [17,30,31], and formation of a ‘graphitized’ tribolayer at the interface, known as ‘friction-induced graphitization mechanism’ [32,33]. Recently, Ma et al. [34] proposed a shear localization mechanism for explaining the superlubricity of DLC films. The passivation of DLC has been demonstrated both experimentally and theoretically. However, only a few studies investigate the rehybridization of tetrahedral amorphous carbon (ta-C) coatings and diamond. The mechanism behind the stick-slip type of friction in hydrogen-free DLC coatings is still unknown. This work is trying to fill these knowledge gaps by investigating the tribological behavior of amorphous carbon using MD simulations. The effects of the carbon bonding network structure and the sp^3/sp^2 ratio of carbon atoms on the tribological properties, e.g., friction force of DLC films, are investigated. In addition, the influence of the hydrogen content on the friction force of amorphous carbon is also studied.

2. Numerical methods

2.1. Empirical potentials

Li et al. [35] presented that empirical potentials have a strong effect on the hybridization and structure of amorphous carbon in MD modeling using liquid quenching method. It is unable to get a greater fraction of sp^3 content more than 20% to use the REBO potential [35]. Therefore, in order to obtain a large sp^3 hybridization fraction of DLC film, the ReaxFF potential is used to model amorphous carbon coatings. By considering computational efficiency and calculation accuracy, the second generation of REBO (2nd REBO) potential, which has been successfully applied to simulate the tribological behavior of amorphous carbon [28,36,37], is employed to investigate the nano-tribological process during sliding.

The 2nd REBO potential was developed by Brenner et al. [36], containing improved analytical functions and an extended database relative to the earlier version [37]. In addition, a long-ranged interaction is considered making the 2nd REBO potential more accurate than its previous version. The detailed information of the 2nd REBO potential is presented below:

$$E_b = \sum_i \sum_{j(j>i)} [V^R(r_{ij}) - b_{ij}V^A(r_{ij})] \quad (1)$$

$$V^R(r) = f^c(r) \left(1 + \frac{Q}{r}\right) A \exp(-\alpha r) \quad (2)$$

$$V^A(r) = f^c(r) \sum_{n=1,3} B_n A \exp(-\beta_n r) \quad (3)$$

$$f_{ij}^c(r) = \begin{cases} \left[1 + \cos\left(\frac{\pi(r - D_{ij}^{\min})}{D_{ij}^{\max} - D_{ij}^{\min}}\right)\right] / 2 & r < D_{ij}^{\min} \\ 1 & D_{ij}^{\min} < r < D_{ij}^{\max} \\ 0 & r > D_{ij}^{\max} \end{cases} \quad (4)$$

where E_b represents the chemical binding energy, and V^R and V^A are pair-additive interactions that represent all interatomic repulsions and attraction from valence electrons, respectively. r_{ij} is the distance between pairs of nearest-neighbor atoms i and j , and b_{ij} is a bond order between atoms i and j . $f_{ij}^c(r)$ is a smoothing cutoff function, having a form shown in Eq. (4). All parameters used in Eqs. (1)–(4) are shown in Table 1.

2.2. Molecular dynamics model

Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software [38] was employed to perform the MD simulation. A schematic diagram of the simulation model is shown in Fig. 1. In this work, the simulation system consists of a counterface and a sample made out of tetrahedral amorphous carbon atoms. The liquid quenching method,

Table 1
Parameters for the carbon-carbon pair terms used in the 2nd REBO [33].

Parameter	Value	Units
$D_{ij}^{\max}$	2.0	Å
$D_{ij}^{\min}$	1.7	Å
A	10953.54	eV
Q	0.31	Å
α	4.75	Å
B_1	12388.79	eV
B_2	17.57	eV
B_3	30.71	eV
β_1	4.72	Å ⁻¹
β_2	1.43	Å ⁻¹
β_3	1.38	Å ⁻¹

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