Wear 372-373 (2017) 12–20

Contents lists available at ScienceDirect

Wear

journal homepage: www.elsevier.com/locate/wear

Wear and friction between smooth or rough diamond-like carbon films and diamond tips

Lichun Bai [a,b], Narasimalu Srikanth [a], Elena A. Korznikova [c], Julia A. Baimova [c], Sergey V. Dmitriev [c,d], Kun Zhou [b,*]

[a] Interdisciplinary Graduate School, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore
[b] School of Mechanical and Aerospace Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore
[c] Institute for Metals Superplasticity Problems, Russian Academy of Sciences, Khalturin St. 39, Ufa 450001, Russia
[d] Research Laboratory for Mechanics of New Peter the Great St. Petersburg Polytechnic University, Polytechnicheskaya St. 29, St. Petersburg 195251, Russia

ARTICLE INFO

Article history:
Received 16 May 2016
Received in revised form
5 December 2016
Accepted 7 December 2016
Available online 8 December 2016

Keywords:
Wear
Friction
DLC film
Molecular dynamics simulation

ABSTRACT

The tribology of diamond-like carbon (DLC) films has been studied for decades, but their friction and wear mechanisms at the nanoscale still remain unclear due to experimental limitations. To address this challenge, the friction and wear between DLC films and diamond tips are investigated via molecular dynamics simulations. It is found that the load can increase wear rate of the DLC film by inducing transition of its wear from adhesive to abrasive type. The calculated friction force follows the prediction of the Bowden-Tabor model at relatively small loads but deviates at large loads due to the formation of transfer layers. The high velocity can decrease the friction force and wear rate of the DLC film by reducing the sliding depth of the diamond tip and number of bonds at the contact interface. When the surface roughness of the DLC film increases, its abrasive wear is highly promoted, leading to the fact that the friction force increases while the wear rate initially decreases and then increases. This surface roughness-dependent wear behavior is attributed to the competition between the adhesive and abrasive wear.

1. Introduction

Diamond-like carbon (DLC) films that are comprised of sp^3 and sp^2 hybridized carbon atoms have been used widely as solid lubricants of workpieces to reduce their surface friction and improve their wear resistance [1]. The excellent tribological behaviors of the DLC film are commonly attributed to its superior mechanical properties and formation of graphitic transfer layers on the surface of counterparts [2]. Many studies have demonstrated that the tribological behaviors of the DLC film highly depend on its surface roughness and working condition [3–5]. However, a fundamental analysis of such dependence is unrealistic in macroscale experiment. This is because the macroscale friction and wear are commonly caused by the contact of surface asperities and their relative sliding [6–12]. These contact and sliding happen at the nanoscale and thus are hardly observed at the macroscale. Therefore, the investigation of nanotribology of the DLC film can help to understand its tribological behaviors.

The molecular dynamics (MD) simulation may help to investigate the nanotribology of DLC films. It has been reported that the friction force F_f at the nanoscale follows the well-known Bowden-Tabor model in which the F_f is linearly proportional to the real contact real area A_{real} which is suitable to be described by the number of bonds n_b at the contact interface [13–15]. Moreover, it has been reported that the nanoscale wear follows the macroscale wear laws in some cases [15,16].

In the present study, the nanotribological behaviors of DLC films are investigated by MD simulations. The influences of the load, velocity and surface roughness are studied.

2. Modelling

The simulation system consists of a diamond tip sliding against a DLC film, as shown in Fig. 1. The sliding is realized by setting the diamond tip with a velocity v_x along the x-direction and a normal load F_n along the z-direction. The periodic conditions of the system are set along the x and y-directions.

The diamond tip that is a half-sphere with a radius of 15 Å is located in the middle of the DLC film along the y-direction. Moreover, this tip is set as a rigid body to keep its geometry unchanged during the simulation. The DLC film has dimensions of $237 \times 42 \times 26$ Å^3. Such film is divided into three layers along the z-direction according to their functions. The bottom layer with a

* Corresponding author.
E-mail address: kzhou@ntu.edu.sg (K. Zhou).

http://dx.doi.org/10.1016/j.wear.2016.12.007
0043-1648/

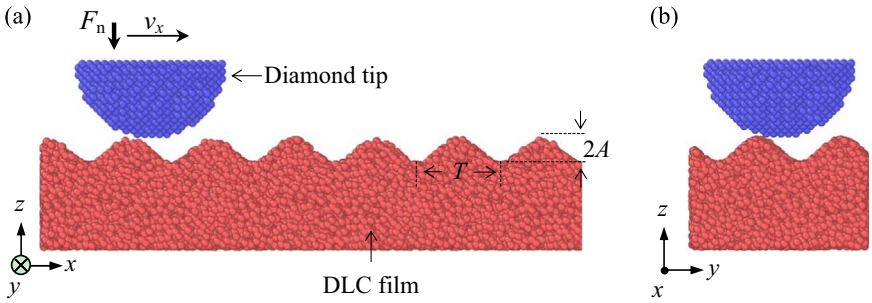

Fig. 1. Configuration of the friction model with (a) a front view and (b) a side view.

thickness of 3 Å is always fixed to keep the DLC film static. The middle layer with a thickness of 3 Å is coupled to a Langevin thermostat to keep a constant temperature at 300 K. The rest that is the top layer keeps in contact with the diamond tip. Atoms in the top layer are free to move according to the forces of their neighbors. More details of the simulation model can refer to our previous studies [17,18].

The DLC film is obtained via a melt-quenching procedure that is commonly employed to obtain amorphous structures. The procedure is comprised of four steps. Firstly, a crystalline diamond block is initially generated with periodic conditions along all the *x*, *y* and *z*-directions in a canonical NVT ensemble at 300 K. The temperature of the block rapidly increase from 300 K up to be above the melting point of crystalline diamond. The high temperature can easily melt the crystalline diamond block. Secondly, the temperature of the block is kept constant for about 20 ps to make the liquid carbon thermostatically equilibrated. Thirdly, the temperature decreases to 300 K with a rate of 1000 K/ps which allows proper relaxations of the amorphous structure. Finally, the residual stress in the block is eliminated by relaxing its amorphous structure in an isothermal–isobaric NPT ensemble at 300 K. More details of the procedure can refer to previous studies [18–20].

The large-scale atomic/molecular massively parallel simulator (LAMMPS) is used to conduct the MD simulations [21]. The interactions between carbon atoms in the simulations are described by the adaptive intermolecular reactive empirical bond order (AIREBO) potential which is able to model both chemical reactions and intermolecular interactions in hydrocarbon systems [22]. Particularly, the long-range dispersive interactions are neglected, since the diamond tip is easily bonded with the DLC film and thus the short-range interactions determine the friction and wear behaviors of the DLC film and its sp^3-sp^2 transitions [23]. The time step of simulations is set as 1 fs, and their molecular visualizations are conducted by using the software OVITO [24].

Prior to the friction simulation, a load F_n (2.9, 29, 145, 203, 246.5 or 290 nN) is maintained on the diamond tip to make it in contact with the DLC film and the contact is to be equilibrated within 30 ps. Following the contact equilibration, the diamond tip starts to slide with a velocity v_x (1, 2, 4 or 8 Å/ps) to realize the friction simulation and the sliding distance is always kept as 160 Å. The surface roughness of the DLC film is generated by tailoring its morphology based on the combinations of two surfaces that are

$$z = A \sin(2\pi x/T) \quad (1)$$

and

$$z = A \sin(2\pi y/T) \quad (2)$$

where A is the amplitude and T is the period. In the simulations, T is always set as 10 Å and A is changed to obtain various surface morphologies which correspond to the root mean square roughness R_q of 0.707, 1.414, 2.122, 3.537 and 4.952 Å, respectively. In particular, the smooth DLC films ($R_q = 0$) are used when considering the influence of v_x and F_n. The v_x is set as 1 Å/ps in the cases with different F_n, and the F_n is kept as 246.5 nN in the cases with various v_x. The F_n and v_x are set as 246.5 nN and 1 Å/ps in the cases with different surface roughness, respectively.

During the friction simulation, the friction force F_f is obtained by calculating the tangential force of the diamond tip along the *x*-direction. The temperature of atoms is evaluated based on its relation with their kinetic energies [25]. The hybridizations states of carbon atoms in the DLC film are characterized by calculating the number of their nearest neighbors within a cutoff length of 2.0 A which corresponds to the position of first minimum in the radial distribution function of amorphous carbon systems described by the AIREBO potential [26]. The fourfold, threefold and twofold carbon atoms are regarded as sp^3, sp^2 and sp bonded, respectively [19].

The number of worn atoms in MD simulations has been only evaluated in few studies [27,28]. Zhong et al. [27] defined the worn atoms as those removed from substrates. Such definition is improper to characterize the wear at the nanoscale, since the nanowear includes not only the removed materials but also all erosions or sideways displacements of atoms from their original position [29]. In particular, this definition is inaccurate to calculate the number of worn atoms at a small load, because in this case these worn atoms are still bonded to the substrate instead of removed from it.

Recently, Hu et al. qualified worn atoms by evaluating their displacements [28]. Such qualification can avoid many limitations of the wear definition discussed above. Therefore, this qualification is employed in this study. In amorphous solids, when wear of one atom happens, it escapes from the surround or bonds of its nearest neighbor atoms. Such escape of the atom needs its minimal displacement of two bond length which may be chosen as the criteria to identify the worn atoms in amorphous solids such as DLC films. Since the maximum bond length in the DLC film is about 2 Å, its atoms with displacements exceeding 4 Å are regarded as worn atoms.

3. Results and discussions

3.1. Contact interface

Fig. 2a shows the effect of F_n on the number of bonds n_b at the contact interface between the diamond tip and the DLC film prior to the sliding of the diamond tip. The n_b increases with the F_n. It is noticed that the increase rate of the n_b is high at a small F_n but decreases at a large F_n. The variation of this increase rate is due to the presence of the interfacial adhesion, which keeps consistent with observations in the models of JKR and DMT [30]. Moreover, it should be noticed that when the F_n approaches to zero, the n_b is nonzero. This nonzero n_b indicates the existence of bonds at the contact interface even at the zero F_n, agreeing well with results in