Lubrication behavior of n-hexadecane on ZnO layer at the nanoscale:A molecular dynamic exploration

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Abstract

In this work, the lubricating models of Cu-Zn alloy with and without the Zinc oxide (ZnO) layer were established. Molecular dynamics (MD) simulation is employed to investigate the lubrication behavior of n-hexadecane on the ZnO layer at the nanoscale. The diffusion of lubricant molecules, and the interaction and stick-slip effect between the friction pairs and the lubricants are systematically explored. The results show that the ZnO layer limits the diffusion of n-hexadecane molecules and the formed lubricating films in the model of the substrate with the ZnO layer are obvious and stable. During the sliding process, ZnO molecules have strong interaction with lubricants molecules and adsorb lubricants molecules on the surface to form adsorption film. The stick-slip effect in the lubricating films generates periodic shear stress and reduces the wear of the friction pair. The ZnO layer causes lubricants molecules to be arranged regularly on the surface into a stable structure to sustain the greater load.

Highlights

- ZnO layer limits the diffusion of n-hexadecane molecules.
- ZnO molecules have stronger interaction with lubricants molecules.
- n-hexadecane gathers and forms adsorption film near the ZnO surface.
- stick-slip effect in the lubricating films reduces the wear.
- lubricants molecules arrange regularly on the ZnO surface to sustain high load.

1. Introduction

Due to its stable oxidation resistance and excellent wear resistance [1–7], ZnO layers have been used as solid lubricating materials to protect the surface of materials in high-precision systems such as data storage, semiconductor devices, and micro-electromechanical systems (MEMS)[8–12]. Chai et al.[13] generated a ZnO layer, which exhibits low friction coefficient and good wear resistance at air condition, on Si substrate using atomic layer deposition.

The wear resistance of the ZnO layer has been proved, while the working conditions of MEMS, which are manufactured based on metals such as Cu-Zn alloys, are relatively harsh, furthermore, the surfaces of the friction parts are easily worn out, resulting in shortening their the service lives [14–16]. In order to reduce the wear of MEMS parts and increase their service lives, liquid lubricants are employed between the friction pair of MEMS. [17–21]. The liquid lubricant can form lubricating film on the surface of the friction pair to effectively reduce the wear of the MEMS parts. Zhai et al.[22] prepared liquid lubricant with nano-diamond as an additive to study the micro-friction between the Cu-Zn alloy and the steel. The results show that the lubricant can strengthen the formation of lubricating film and significantly reduce the surface wear of Cu-Zn alloy. Bolutife et al.[23] used the metal organic vapor deposition method to obtain an n-doped ZnO layer on the surface of 304L stainless steel. The friction behavior of the ZnO layer and 304L stainless steel substrate was evaluated using a ball-on-disk Micro-Tribometer. The results show

that, under the condition of marginally lubricated, the wear resistance of the n-doped ZnO layer is better than that of the substrate. The ZnO layer has an obvious protective effect on the surface of 304L stainless steel.

On the condition that the lubricant film is in the micro-nanoscale, the physical properties change greatly. In this case, many macroscopic tribological theories are no longer applicable, moreover, it is difficult to explore the mechanism of film lubrication by the experimental method. Therefore, the MD simulation method was employed to investigate the evolution of atomic motion and deeply reveal the characteristics and internal mechanisms of nanostructures. The MD simulation has been widely used in the study of micro-friction behavior at the micro-nanoscale. Song et al.[24] established MD models of the Polytetrafluoroethylene (PTFE) sliding against copper (Cu) substrate under dry friction and water lubrication, respectively. The average friction coefficient of PTFE decreases from 0.189 to 0.064 under water lubrication, which dramatically reduces the wear of PTFE compared with that of dry friction. Hu et al.[25] performed MD simulation to study friction property differences between base fluids and nanofluids during the shear sliding. The results show that, with the increase of load, liquid-solid transitions take place for both base fluids and nanofluids. Specifically, the nanofluids show excellent friction-reducing properties, furthermore, the nanofluids have a higher load-bearing capacity than that of base fluids. Presently, ZnO has been widely studied and applied as a wear-resistant material, however, in the micro-nanoscale, the interaction between ZnO and lubricating fluid, especially the micro-lubrication mechanism under lubricating conditions, has not been effectively explored.

In this work, MD simulation is employed to investigate the lubrication behavior of Cu-Zn alloy coated with the ZnO layer under n-hexadecane fluid lubrication. By comparing the dynamic distribution characteristics of the lubricating fluid during the sliding process of the Cu-Zn alloy with and without the ZnO layer, the interaction between the ZnO and the lubricating fluid was clarified. On this basis, the micro-lubrication behavior between the ZnO and the lubricating fluid at the microscale was revealed.

2. Simulation Procedure And Method

2.1 Analytical theories

In this work, the mean square displacement (MSD) is employed to describe the diffusion of n-hexadecane molecules overtime during the sliding process. The MSD is defined as the collective average of all molecular displacements at a certain moment, furthermore, it is a general measure of molecular diffusion in space[26–28]. In MD simulations, the MSD results illustrate the diffusion trend of lubricants molecules over time. During the sliding process, each lubricating molecule is considered to move continuously from the initial sliding position. The formula is as follows[29].

$$MSD = \Delta r^2(t) = 1/N \sum_{i=1}^{N} [r_i(t) - r_i(0)]^2$$

1

where N is the number of the atoms, i is the i-th atom, and $r_i(t)$ is the position of the atom at time t, respectively.

Radial distribution function (RDF) is a common mathematical function to describe the microstructure of liquid and amorphous materials. The RDF formula is as follows[29].

$$g(r) = 1 \Big/ \rho 4\pi r^2 \delta r \frac{\sum_{i=1}^{t} \sum_{j=1}^{N} \Delta N(r \to r + \delta r)}{Nt}$$

2

where N is the total number of atoms, t is the total simulation time (or step length), δr is the set distance difference, ΔN is the number of atoms between r and $r + \delta r$, respectively.

RDF is used to investigate the structure of molecular systems and the interaction between ZnO molecules and lubricants molecules in this work. In order to verify whether the phase transition of the lubricating fluid occurs during the sliding process, the coordination number of the fluid molecule is calculated [30, 31]. It is integrated with the first peak coordinate of the RDF as the upper limit to obtain the coordination number of surrounding atoms around the central atom. The formula is as follows.

$$N_B = 4\pi \int_0^{R_{\min}} \rho_B g(r) r^2 dr$$

3

where ρ_B is the average number density of surrounding atoms in the entire simulation system. The integral limit is from $R = 0$ to the position $R_{\min}$ of the first peak point of the RDF.

2.2 Models and parameters

The MD simulations were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)[32]. In MD simulations, to reduce the influence of different branches in the sliding process of the hexadecane isomers, n-hexadecane (C16H34) was used as the base fluid of lubricant molecules. The ZnO layer is prepared on the substrate with a hexagonal wurtzite structure, which builds along the (0 0 1) crystal plane[33]. The occupied layers of the zinc atoms and oxygen atoms for the wurtzite structure ZnO are staggered, therefore, the wurtzite configuration of ZnO produces two crystal planes perpendicular to the(0 0 1) crystal plane [34]. The positively charged zinc polar plane composed of zinc atoms is denoted as [0 0 0 1] plane. The other crystal plane species is a negatively charged oxygen polar plane composed of oxygen atoms, denoted as [0 0 0–1] plane[35].

The positively charged zinc polar plane served as the friction pair surface to contact the lubricants molecules. The (0 0 1) crystal plane of the ZnO unit cell was selected to simulate the growth direction of

the ZnO layer in the investigation. Figure 1 (a) shows the ZnO unit cell. The ZnO molecular layers are built along the (0 0 1) crystal plane. Figure 1(b) shows the surface model of ZnO along the growth direction. The surface shown in Fig. 1 (c) is the zinc pole surface [0 0 0 1].

Table 1
Atomic Lennard-Jones parameters used in the MD simulations

Atom	σ(Å)	ϵ(kcal/mol)
C-H		
CH_2	3.93	0.0933
CH_3	3.93	0.2264
WALL		
Zn	2.741	4.679
Cu	3.04	6.47
O	2.96	0.210

Lennard-Jones (LJ) potential 12 − 6 was employed to describe the non-bonded interaction between n-hexadecane molecules, moreover, the mixed potentials including Coulomb potential and LJ 12 − 10 potential were used to pay electrostatic and van der Waals interaction between the n-hexadecane molecules and the ZnO molecules, respectively[36–38]. The force field of the embedded atom method (EAM) was used to describe the interaction between metal atoms, moreover, the parameters of the force field were obtained from the LAMMPS program. The parameters of the LJ potential function are shown in Table 1[39]. Figure 2 (a) and Fig. 2 (c) show the lubrication model of Cu-Zn alloy without and with ZnO layer, respectively. The n-hexadecane fluid is a fully relaxed lubricating fluid medium, as shown in Fig. 2 (b). Under the same conditions of Fig. 2 (a) and Fig. 2 (b), the fully relaxed n-hexadecane is filled between the friction pairs of the two models. During the sliding process, periodic boundary conditions were applied to the model in the *x* and *y* directions, in addition, limited boundary conditions were applied in the *z*-direction. A Langevin thermal bath of 300 K was applied, where the constant temperature layer was reset every 50 steps. The simulation system was prepared ready after full relaxation. With NVT ensemble constrained, the upper friction pair was pulled to move along the positive direction of the *x*-axis at a speed of 0.02 Å/ps. The main parameters of the models are shown in Table 2. The time steps of all simulations are 1.0 fs, and the cutoff radius is 15.0 Å.

Table 2
Parameters used in MD

Projects	Parameters
Dimensions (Å)	$l_{y1}=l_{x1}=32.53$ $l_{z1}=81.60$ $l_{y2}=l_{x2}=32.28$ $l_{z2}=94.70$
Time steps (fs)	1.0
Cutoff distance (Å)	15.0
Alkane type	n-hexadecane
Boundary	p p f

3. Results And Discussion

3.1 MSD and relative concentration

The relationship between the MSD of n-hexadecane molecules and time is shown in Fig. 3, which is used to characterize the diffusion of lubricant molecules during the sliding process of two friction pairs from the initial position to complete separation. Compared with the MSD value of the n-hexadecane molecule in the model of the substrate without ZnO layer, the MSD value in the model of the substrate with ZnO layer is smaller under the same simulation conditions. It means that the n-hexadecane molecules in the model of the substrate without ZnO layer show a more intense degree of diffusion than that of the model of the substrate with ZnO layer under the same conditions. Although the n-hexadecane molecules still exhibit diffusivity characteristic in the model of the substrate with ZnO layer, it is obvious that the ZnO layer limits the diffusion of n-hexadecane molecules. In addition, during the sliding process, the n-hexadecane molecule maintains a high degree of order and a low degree of dispersion under the internal action of ZnO layer.

The dispersion characteristics of lubricants molecules, which are in the two models of the substrates with and without ZnO layer, can be obtained through the relative concentration curve. Figure 4 and Fig. 5 exhibit the relative concentration changes of n-hexadecane lubricants molecules in the two models of substrates with and without ZnO layer during the sliding process. The relative concentration curves of n-hexadecane molecules in two Figs both have obvious peaks close to the surfaces of friction pairs and fluctuate slightly during sliding processes. These phenomenons indicate that the n-hexadecane molecules aggregate and form lubricating films on the upper and lower surfaces of friction pairs. 7 different values of relative concentration, which are the peaks in the curve, are obtained in the model of the substrate without ZnO layer in Fig. 4, while only 6 different values of relative concentration are obtained in the model of the substrate with ZnO layer in Fig. 5. These phenomenons mean that, during the sliding process, the lubricating fluids are divided into 7 and 6 lubricating films in two models, respectively.

As shown in Fig. 5, the thickness of lubricating films, which is about 25 Å, in the model of the substrate with ZnO layer is thinner than that of, which is about 31 Å, in the model of the substrate without ZnO layer. Furthermore, in the model of the substrate with ZnO layer, the relative concentration of lubricating films close to the surfaces of two friction pairs is about 4.3 and 4.7, respectively. The relative concentration of the other four lubricating films, which are in the middle of the curve, remains stable at around 3.5 and oscillates between 3.2 and 4.2 with distance. Comparing the curve of lubricating films in the model of the substrate without ZnO layer, in the model of the substrate with ZnO layer, the values of peak maintain higher, and meanwhile have smaller fluctuations during the sliding process. It illustrates that the distribution of n-hexadecane molecules in the model of the substrate with ZnO layer is relatively uniform and stable with considerably smaller scatter in the value of migration in the z-direction with time. In Fig. 4, the values of the peak are lower in the middle of the curve with fluctuating around three insignificant peaks. These results indicate that the formed lubricating films are not obvious and unstable in the model of the substrate without ZnO layer.

It is observed that the relative concentration close to the upper and lower surfaces in Fig. 5 fluctuates smaller with time. The phenomenons mean that the lubricating films, which are close to the upper and lower surfaces, spread and slid at the same speed with the friction pair sliding. These two lubricating films are called adsorption films, which adsorb on the surface of friction pair. Based on the curves in Fig. 4 and Fig. 5, the lubricating films maintains stability during the sliding. Actually, during the sliding process, the interface molecular film has three different physical statuses, which are solid-like, amorphous, and liquid-like[40]. Based on classical fluid mechanics theory the strong adsorption force of alkane molecules on the upper and lower surfaces can make lubricating film showing solidity, forming a thick solid adsorption film to participate in shear lubrication, and meanwhile, the adsorption force limits the spread of alkanes[41]. Therefore, to analyze the interaction effect between the lubricants molecules and ZnO layer, the interaction distance between them needs to be investigated.

3.2 RDF and coordination number

Figure 6 draws the RDF curves of the interaction distance between the lubricating molecules and the surface molecules of the friction pair in the models of the substrate with and without ZnO layer, respectively. The abscissa r represents the interaction distance between the surface molecules and the lubricants molecules. In the two curves, the peaks and valleys are observed significantly. Initially, the RDF values are all zero with $r < 0.75$Å. Afterward the curves steeply sharp to the maximum values at the first peak, $r = 2.25$ Å. It implies that a large number of n-hexadecane molecules gather near the surfaces of friction pairs at $r = 2.25$ Å, meanwhile, ZnO molecules on the surface of the friction pair polarize the n-hexadecane molecules close to the surface. The density of lubricants molecules near the peaks is much higher than the average density of the curves. The deep valleys, which represent the weak interaction areas, between the two peaks are observed in the curves. The second peaks of both curves represent the medium degree of connection strength. For the model of the substrate without ZnO layer, the values of the RDF curve are generally smaller than the values of the RDF curve obtained in the model of the substrate with ZnO layer.

Molecular aggregations are caused by the distance of molecules reducing, and moreover, a smaller distance from the reference atom means a stronger aggregating degree of molecules. Compared with copper and zinc atoms, ZnO molecules have stronger interaction with lubricants molecules, enabling the lubricants molecules to exist in a more compact form on the surfaces during the sliding process. The curves abscissa corresponds to the interaction distance between the surface molecules and the lubricants molecules. In Fig. 6, the first peaks of the curves indicate that the distance between the lubricating films near the surface and the surface is all 2.25 Å. For the model of the substrate without ZnO layer, the second peak in the curve is smooth, furthermore, to the end of the curve, the curve shows the weak interaction between the Cu-Zn alloy molecules and the lubricants molecules.

The coordination number is used to measure the number of n-hexadecane molecules surrounding the surface of the friction pair. The coordination number not only reflects the binding ability and coordination relationship between lubricants molecules and the surface molecules, but also describes the tightness of the lubricants molecules during the sliding process. The larger the coordination number means the tighter molecules arrangement. According to formula (3), the position of the first peak of the RDF in Fig. 6 is R_{min}=2.25 Å, furthermore, the number of carbon atoms in the adsorption films, which are on the two kinds of friction pair surfaces, was calculated to characterize the tightness of n-hexadecane molecules. For the substrates with and without ZnO layer, the coordination numbers are 119.4 and 91.4 respectively. It can be obtained that the carbon atoms of n-hexadecane gathered in the lubricant films, which are the closest to the surfaces of substrate with ZnO layer, is about 1/4 of the total number of the simulated carbon atoms in the adsorption film. Furthermore, this coordination number is about 1.3 times that of the model of the substrate without ZnO layer. According to the RDF image and coordination number results, the ZnO layer leads to more n-hexadecane molecules gathering near the friction surface to form adsorption film, which proves the result of Fig. 5. Due to the hydrogen bond and van der Waals interaction with the ZnO molecules, adsorption film adsorbs on the surface of ZnO layer, moreover, the adsorption capacity decreases with the increasing distance from the surfaces. Figure 7 shows the snapshot of the sliding process in the model of the substrate with ZnO layer and the sketch of films movement during the sliding process, respectively. Figure 7(a) exhibits that, in the model of the substrate without ZnO layer, the lubricants protect the friction surface and are subjected to shear stress during the sliding process. Figure 7(b) is the schematic diagram of lubricating films movement during the sliding process. The lubricating films are arranged in parallel in the film thickness direction and maintain the same movement direction. Therefore, the transmitting motion behavior of lubricating films, which include adsorption film, needs to be investigated in detail.

3.3 Shear stress

Based on the above results, the interaction between the n-hexadecane molecules and the surface of the friction pair belongs to physical adsorption behavior. During the sliding process, the lubricating films separate the two surfaces of the friction pair, meanwhile, the friction force is caused by conquering the shear stress between the two surfaces. Adsorption film adsorbs on the surface of friction pair to participate in the sliding. Figure 8 shows the shear stress on the upper and lower surfaces of the friction

pair of the model without ZnO layer during the sliding process. It is observed that the stresses on the upper and lower surfaces maintain and fluctuate near their own fixed values of the vertical axis, respectively. Similar phenomenons are shown in Fig. 9 (a), which is the shear stress change on the upper and lower surfaces of the friction pair of the model with ZnO layer during the sliding process. However, the overall shapes of stress curves in Fig. 9 (a) show more regular than these in Fig. 8. By observing the enlarged curves in Fig. 9 (b), during the sliding process, the shear stresses fluctuate regularly within a certain range and exhibit periodic characteristics. The stick-slip effect, which is caused by the interaction of molecules, between the friction pairs and the lubricating films leads to a regular curve shown in Fig. 9 (a), and moreover, the hilly bulge area on the shear stress in Fig. 9 (a) is the significant feature of the stick-slip effect. During the process of the lubricating films from adhesive contact to the beginning of sliding, the shear stress gradually increases from the minimum dynamic shear stress to the maximum static shear stress, then the lubricating film molecules begin to slide and enter a new adhesive contact with the friction pair surface, and meanwhile, the shear stress gradually decreases to the minimum dynamic shear stress. During the sliding process, the alternate adhesion and sliding of the lubricating films reduce the wear of the friction pair. Comparing the shear stress curves in Fig. 8 and Fig. 9(a), it is inferred that the ZnO layer on the friction surface causes periodic shear stress and maintains a stable stick-slip effect, which results in a firm adsorption molecular film structure and a strong interaction between the surface and lubricants.

Based on the result of Fig. 6, the strong polarity, which is between the ZnO lubricants on the surface of the friction pair and the n-hexadecane molecules, leads to the strong interaction between the surface and lubricants. With the combined effect of Van der Waals force and electrostatic force, lubricants molecules form lubricating films during the sliding, which are shown in Fig. 10(a). Between these lubricating films, low concentration cavities are generated due to the lubricants molecules gathering up or down to the lubricating films. The polar molecules in the lubricating film are arranged in regular order on the surface of the film. During the sliding process, the polar molecules on two adjacent lubricating films contact and slide with each other to produce the stick-slip effect. With the action of the stick-slip effect, the polar molecules in one lubricating film transfer the motion to the next lubricating film, resulting in periodic shear stress as shown in Fig. 9 (b).

Figure 10 (b) shows the arrangement state of n-hexadecane molecules in the model of the substrate with ZnO layer. The results of the coordination number indicate a large number of lubricants molecules in adsorption film are aggregated on the surface of the substrate with ZnO layer. Therefore, compared with lubricants molecules adsorbed the surface of the substrate without ZnO layer (Fig. 10 (a)), more lubricants molecules are aggregated and bear the load on the surface of the substrate with ZnO layer. Figure 11 describes the change of pressure on the surface of the substrate. The pressure on the surface of the substrate with ZnO layer drops at the sliding start, and then stabilizes at about 2.4Gpa finally, and meanwhile, the pressure values on the surface of the substrate with ZnO layer are higher than that on the surface of the substrate without ZnO layer. Under the same sliding conditions, the ZnO layer causes lubricants molecules to be arranged regularly on the surface into a stable structure, which sustains greater loads.

4. Conclusions

(1) The ZnO layer limits the diffusion of the n-hexadecane molecules during the sliding process. The thickness of lubricating films in the model of substrates with and without ZnO layer is about 25 Å and 31 Å, respectively. The lubricating fluids in the two models are divided into 7 and 6 lubricating films, respectively. The formed lubricating films in the model of the substrate with ZnO layer are obvious and stable.

(2) The RDF curves indicate that the ZnO molecules have stronger interaction with lubricants molecules, furthermore, the strength of the interaction decreases with distance. According to coordination number results, the ZnO layer leads to more n-hexadecane molecules gathering near the friction surface to form stable adsorption film.

(3) Due to the effect of adsorption film on the surface of friction pair with ZnO layer, the shear stresses fluctuate regularly within a certain range and exhibit periodic characteristics. The stick-slip effect in the lubricating films reduces the wear of friction pair. In addition, the ZnO molecules cause lubricants molecules adsorbing and regular arranging on the surface to sustain greater loads.

Declarations

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Figures

Figure 1

ZnO unit cell and molecular layer view.

Figure 2

(a) Lubrication model of Cu-Zn alloy without ZnO layer, (b) n-hexadecane fluid, (c) Lubrication model of Cu-Zn alloy with ZnO layer

Figure 3

Relationship between MSD and simulation time

Figure 4

Lubricants molecules relative concentration in thickness direction (substrate without ZnO layer)

Figure 5

Lubricants molecules relative concentration in thickness direction (substrate with ZnO layer)

Figure 6

RDF of hexadecane in the presence or absence of ZnO layer

Figure 7

(a) Snapshot of sliding process in model of substrate with ZnO layer, (b) Sketch of lubricating films movement during the sliding process.

Figure 8

Shear stress on the upper and lower surfaces of friction pair of substrate without ZnO layer.

Figure 9

(a) Shear stress on the upper and lower surfaces of friction pair of substrate with ZnO layer, (b) Magnified image of shear stress area.

Figure 10

(a) Arrangement state of n-hexadecane molecules in the model of substrate without ZnO layer, (b) Arrangement state of n-hexadecane molecules in the model of substrate with ZnO layer

Figure 11

Pressure on the surface of substrates