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 lubricants 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.

Keywords Molecular dynamics · Lubricating film · Stick–slip effect · ZnO layer · N-hexadecane

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 its 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 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 lubricants can form adsorption films on the surface of the friction pair to effectively reduce the wear of the MEMS parts. Zhai et al. [22] prepared liquid lubricants with nano-diamond as an additive to study the micro-friction between the Cu–Zn alloy and the steel. The results show that the lubricants 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 lubricating 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 sliding shear. The results showed 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 over time 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 lubricants molecule is considered to move continuously from the initial sliding position. The formula is as follows [29].

\[
MSD = R(t) = \left( \frac{1}{N} \sum_{i=1}^{N} (r_i(t) - r_i(0))^2 \right)^{1/2},
\]

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. The RDF formula is as follows [29].

\[
g(r) = \frac{1}{\rho V_{l} r^2} \left( \frac{1}{\delta r N_t} \sum_{i=1}^{N} \sum_{j=1}^{N} \Delta N(r \rightarrow r + \delta r) \right),
\]

where \(N\) is the total number of atoms, \(t\) is the total simulation time (or step length), \(\delta r\) is the set distance difference, and \(\Delta N\) 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 valley coordinate of the RDF as the upper limit to obtain the coordination number of surrounding atoms around the central atom. The formula of coordination number is as follows.

\[
N_B = 2\pi \frac{N_L}{V_L} \int_{0}^{R_{\text{min}}} g(r) r^2 dr,
\]

where \(V_L\) is the lubrication volume, \(N_L\) is the number of atoms of n-hexadecane lubricating molecule with C as the characteristic atom in the lubricating volume, \(g(r)\) is radial distribution function, \(r\) is the cutoff radius, and \(R_{\text{min}}\) is the abscissa of the first valley of the radial distribution function, respectively.

### 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 lubricants molecules. The ZnO layer is prepared on the Cu substrate with a hexagonal wurtzite structure, which builds along the (0 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 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 0 1) crystal plane of the ZnO unit cell was selected.
to simulate the growth direction of the ZnO layer in the investigation. Figure 1a shows the ZnO unit cell. The ZnO molecular layers are built along the (0 0 0 1) crystal plane. Figure 1b shows the surface model of ZnO along the growth direction. The surface shown in Fig. 1c is the zinc pole surface (0 0 0 1).

The intra-molecular interactions of n-hexadecanes were described by the COMPASS force field. The formula of COMPASS force field is as follows [36–38].

\[
U_{\text{total}} = U_{\text{band}} + U_{\text{angle}} + U_{\text{torsion}} + U_{\text{oop}} + U_{\text{cross}} + U_{\text{elec}} + U_{\text{LJ}},
\]

where \( U_{\text{band}} \), \( U_{\text{angle}} \), \( U_{\text{torsion}} \), \( U_{\text{oop}} \), \( U_{\text{cross}} \), \( U_{\text{elec}} \), and \( U_{\text{LJ}} \) represent the contributions of bond stretching, angle bending, torsion angle, out-of-plane angle coordinates, cross-coupling, electrostatic, and van der Waals interactions, respectively.

The Lennard–Jones potential (LJ) 12–6 was employed to describe the non-bonded interaction including between n-hexadecane molecules, and between substrate surface and n-hexadecane molecules. The formula of LJ 12–6 is as follows [38].

\[
u_{\text{LJ}}(r_{ij}) = 4\varepsilon_{ij}\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - 2\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6},
\]

where \( r_{ij} \) is the intermolecular distance between atoms \( i \) and \( j \), and \( \varepsilon_{ij} \) and \( \sigma_{ij} \) are the energy parameter and the length scale of atoms \( i \) and \( j \), respectively.

The Lennard–Jones parameters of n-hexadecane molecules and the ZnO surface are shown in Table 1. The interaction between C-H and surface atoms is calculated by the Lorentz-Berthelot mixing rule. The Lorentz-Berthelot rules allow the mixing of the Lennard–Jones parameters [38].

\[
\sigma_y = \frac{1}{2}(\sigma_{ii} + \sigma_{jj}) \quad \text{and} \quad \varepsilon_y = \sqrt{\varepsilon_{ii}\varepsilon_{jj}},
\]

where \( \varepsilon_{ij} \) and \( \sigma_{ij} \) are the energy parameter and the length scale of atoms \( i \) and \( j \), respectively.

The interactions between metal atoms (Cu–Cu, Cu–Zn) were described by embedded atom method (EAM) potential [43, 44]. The atom interactions of ZnO (Zn–Zn, Zn–O, O–O) were also described by EAM potential, moreover, the potential parameters were developed by Erhart et al. [45].

Figure 2a and c show the lubrication model of Cu–Zn alloy without and with ZnO layer, respectively. The atom number of Cu–Zn alloy in Fig. 2a and c are the same, moreover, the ZnO layers are generated on the surface of Cu–Zn alloy model in Fig. 2c. As shown in Fig. 2b, the density and number of lubricants molecules, which is n-hexadecane in every model box, are 0.7 g/cm³ and 60, respectively. The periodic boundary conditions were applied to the model in the \( x \) and \( y \)-axis, in addition, limited boundary conditions were applied in the \( z \)-axis. A Langevin thermal bath of 300 K was applied, where the constant temperature layer was reset every 50 steps. After full of relaxation, the simulation systems were prepared ready with a surface pressure of 0.5 GPa. With the NVT ensemble constrained, the upper friction pair was pulled to move along the direction of the \( x \)-axis at a speed of 0.2 Å/ps [37].

### Table 1 Parameters of Lennard–Jones 12–6

| Atom       | \( \sigma (\text{Å}) \) | \( \varepsilon (\text{kcal/mol}) \) |
|------------|-------------------------|-----------------------------------|
| Lubricants |                         |                                   |
| CH₂-CH₂   | 3.93                    | 0.09                              |
| CH₃-CH₃   | 3.93                    | 0.23                              |
| Surface   |                         |                                   |
| Zn-Zn     | 2.74                    | 4.68                              |
| Cu-Cu     | 3.04                    | 6.47                              |
| O-O       | 2.96                    | 0.21                              |

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### 3 Results and Discussion

#### 3.1 MSD and Relative Concentration

The MSD curves are used to characterize the diffusion of lubricants molecules. The relationship between the MSD of n-hexadecane molecules and time is shown in Fig. 3. It can be obtained that the slope of the MSD tends to stabilize after the time of 1000 ps. The stable MSD value in the model with ZnO layer and without ZnO layer are 0.32 and 0.53, respectively. 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 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. Figures 4 and 5 exhibit the relative concentration changes of n-hexadecane lubricants molecules in the two models of substrates without and with ZnO layer during the sliding process. The relative concentration curves of n-hexadecane molecules in two figures both have obvious peaks close to the surfaces of friction pairs and fluctuate.
slightly during sliding processes. These phenomena indicate that the n-hexadecane molecules aggregate and form adsorption 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 phenomena mean that, during the sliding process, the lubricating fluids are divided into 7 and 6 lubricating films in two models, respectively.

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 4.5, 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 3.8 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 overall 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 phenomena mean that the lubricating films, which are close to the upper and lower surfaces, spread and slide 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 Figs. 4 and 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 [46]. 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 [47]. 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 peak values of the RDF curve are generally smaller than that of 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 absissa 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 valley of the RDF in Fig. 6 is \( R_{\text{min}} = 4.25 \, \text{Å} \). 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 n-hexadecane molecules, which are calculated by coordination numbers, are 15 and 8, respectively. It can be obtained that the molecules of n-hexadecane gathered in adsorption film, which is the closest to the surfaces of the substrate with ZnO layer, are about 1/4 of the total number of the simulated n-hexadecane molecules. Furthermore, the number of n-hexadecane molecules in adsorption film of the substrate with ZnO layer is about 1.87 times that 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 velocity in the thickness direction of lubricants, respectively. Figure 7a 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. The sliding velocity of lubricating films in different positions along the z-axis direction is shown in Fig. 7b. During the sliding, the lubricating films in lubricants maintain the same movement direction with the up substrates of the two models. The velocity value of the lubricating films decreases from the upper substrate surface to the lower substrate surface, furthermore, the velocity values of the lubricating films in the model with ZnO layers are greater than that of the model without ZnO layers.

Figure 8b shows the arrangement state of n-hexadecane molecules in the model of the substrate with ZnO layer. The

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**Fig. 7**: a) Snapshot of sliding process in model of substrate with ZnO layer, b) Velocity in the thickness direction of lubricants
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 on the surface of substrate without ZnO layer (Fig. 8a), more lubricants molecules are aggregated on the surface of the substrate with ZnO layer. Additionally, 6 lubricating films are more clearly observed in Fig. 8b, which is consistent with the results obtained in Figs. 4 and 5.

### 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 9 shows the shear stress, which is calculated according to Ref.[48], 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 phenomena are shown in Fig. 10a, 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. 10a shows more regular than these in Fig. 9. By observing the enlarged curves in Fig. 10b, 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. 10a, and moreover, the hilly bulge area on the shear stress in Fig. 10a 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. Comparing the shear stress curves in Figs. 9 and 10a, 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. 8b. 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 regularly 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 shown in Fig. 10b.

4 Conclusions

(1) The ZnO layer limits the diffusion of the n-hexadecane molecules during the sliding process. 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. In addition, the ZnO molecules cause lubricants molecules to adsorb and regular arranging on the surface.

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Declarations

Conflict of interest The authors have not disclosed any competing interests.

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