Achieving Macroscale Liquid Superlubricity Using Lubricant Mixtures of Glycerol and Diols

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Abstract

Friction and wear are ubiquitous in moving mechanical systems, and achieving vanishing friction and wear could significantly improve energy efficiency and extend the service life of mechanical components. In this paper, various diols, *viz.* ethylene glycol (EG), 1,3-propanediol (13-PD), and 1,2-propdiol (12-PD), have been selected to be mixed with glycerol for superlubricity performance. The results show that the lubricant mixture of EG and glycerol (EG/glycerol) and the mixture of 13-PD and glycerol (13-PD/glycerol) are effective in providing superlow friction ($\text{COF} < 0.01$) for steel tribopairs under ambient atmosphere environment with little surface damage caused. However, 12-PD, which exhibits the same chemical formula as 13-PD except for the configuration of hydroxyl groups, is ineffective for superlubrication. Furthermore, compared with 13-PD, EG is more efficient in preparing superlubric lubricants. Experimental and molecular dynamics simulation results show that the superlow friction realized by the lubricant mixtures of glycerol and diols is related to their intermolecular hydrogen-bonding interaction and the adsorbed formation of adsorbed molecular layers. The intermolecular interaction could affect the rheological property of lubricant mixtures and the hydrodynamic lubricant film-forming capability at the interface, while the quality of the adsorbed molecular layers determines the passivating efficiency for asperity interactions between opposite surfaces. Due to the atomic structure difference, EG is the most desirable diol for this objective, followed by 13-PD, while 12-PD is ineffective. These findings could help enable the rational design of novel lubricants for superlubricating performance and push the development of liquid superlubricity for future engineering applications.

1. Introduction

Superlubricity with vanishing friction is promising to solve energy dissipation and prevent premature working components failure induced by friction and wear. It is estimated that 23% of the world's total energy is consumed by tribological contacts, and the implementation of advanced surface treatment techniques, novel base materials, and innovative lubricants could potentially reduce the energy loss by 40% [1]. Fulfilling this goal requires precise manipulation of friction and wear behavior. Researchers have paid lots of efforts to explore the origin of friction, and several factors, including contact adhesion, interfacial bonding, viscous dissipation, and microstructure evolution, have been interpreted to be the main causes [2-7]. Precisely tuning these factors sheds light on achieving controlling friction or even realizing vanishing friction.

The atomistic origin of friction under various dimensionality has been researched by Hirano in the 1990s, in which he predicts that achieving vanishing friction is possible at high dimensionality when two conditions are met: the adiabatic motion of atoms and the phenomena of energy recurrence [8-10]. He indicated that these two conditions could be satisfied by using two clean flat crystalline surfaces that engage an incommensurate orientation, where forces acting on each atom could cancel out [10, 11]. Up to now, this hypothesis has been experimentally demonstrated within molybdenum disulfide sheets, graphene sheets, carbon nanotubes, and some heterogeneous structures in micro/nanoscale under a vacuum atmosphere [12-16]. However, in real applications, the reactive species of oxygen and water in the

air and the defects of materials could enhance the interfacial interaction and cut off the stable sliding area, which could lead to the non-adiabatic motion of atoms and continual energy dissipation, hindering the occurrence of vanishing friction phenomenon.

Liquid lubricated systems could partially or even totally separate the solid contacts by generating thin pressurized lubricant films, remarkably alleviating the severity of friction. The overall friction for a liquid lubricated system comes mainly from two sources: the viscous dissipation of lubricant films and the adhesive interaction between opposite asperities [17]. The former could be controlled through viscosity manipulation, while the latter can be minimized by the adsorption of molecular layers of lubricant molecules. Recently, hydration lubrication has emerged as a promising strategy to macroscale liquid superlubricity, where water molecules are kept by charges surrounding ions or polar molecules, which still maintains flexibility like liquids and remains integrity under pressure [18-23]. Furthermore, both water and polar molecules could attach to the steel surface to minimize the interfacial bonding. One drawback of this approach is that it requires hundreds of seconds long wearing-in before transiting to the vanishing friction state, with serious materials loss caused [24]. Though adding nanoparticles in lubricants could reduce wear to an extent, it does not fundamentally solve the issue and the long wearing-in still exists [25].

In our study, as displayed in Figure 1, glycerol is employed as the base liquid lubricant, mixing with three different diols, *viz.* ethylene glycol, 1,3-propanediol, and 1,2-propanediol, pursuing stable and robust superlubricating ability. Experiments have been designed to test the rheological properties of the lubricants and their tribological performances. Molecular dynamics simulation is used to explain the behaviors of lubricant molecules at the atomic scale, including the intermolecular interaction between lubricant molecules, distribution of lubricant molecules across the surfaces, and the interaction between lubricant molecules and friction surfaces. The selection of diols provides us an opportunity to explore how the modification of molecular structures of diols would affect the friction behavior, providing a guideline to the future tailored design of lubricants with superlubricity performance.

2. Material And Methods

2.1 Experimental details

Glycerol (purity = 97%), 1,3-propanediol (13-PD, purity = 99%), and 1,2-propanediol (12-PD, purity = 99.5%) were purchased from Alfa Aesa, while ethylene glycol (EG, purity = 97%) was from J. T. Baker. Lubricant mixtures of diol and glycerol (diol/glycerol) were prepared by mixing diol with glycerol at various diol/glycerol weight ratios, *viz.*, 0.2, 0.4, 0.6, and 0.8. Further ultrasonication process was carried out to make the mixtures uniform. For simplicity, the prepared mixtures were labeled according to their diol/glycerol weight ratio: EG/glycerol = 0.2, 0.4, 0.6, and 0.8; 13-PD/glycerol = 0.2, 0.4, 0.6, and 0.8; 12-PD/glycerol = 0.2, 0.4, 0.6, and 0.8. Steel disk and ball made of AISI 52100 steel were used as tribopairs. The ball diameter is 9.5 mm and its surface roughness R_q is 20 nm. The diameter and height of the disk are 30 mm and 5 mm respectively, and its surface roughness R_q was polished to be about 20 nm.

The kinetic viscosity of lubricants was measured by Cannon-Fenske Routine Viscometer, with the environmental temperature controlled at 25 °C by CANNON CT-2000 Extended Range Constant Temperature Bath. Lubricant density was further experimentally determined. The corresponding dynamic viscosity was obtained by multiplying the kinetic viscosity of lubricants with their densities.

Tribotests were carried out on CETR UMT-2 ball-on-disk tribometer. The wear track diameter and the rotation speed were maintained at 12 mm and 159.23 rpm respectively, corresponding to a linear speed of 0.1 m/s. The applied load was adjusted from 4 to 7 N, with the calculated Hertz contact pressure of 723 - 871 MPa. The testing duration was 30 min. Repeat tests have been conducted, which showed great reproducibility. After the test, tribopairs were rinsed with methanol to remove the residual lubricant. The surface morphology of steel surfaces was characterized by Laser Confocal Microscope (Bruker). The deposit formed on the ball surface was analyzed by Horiba Raman, where a 473 nm laser source was employed.

2.2 Computation details

Molecular dynamics (MD) simulation was conducted on LAMMPS, which is a widely used large-scale atomically massively parallel simulator [26]. The Reactive force field (ReaxFF) that has been validated for hydrocarbon analysis was employed [27]. The open visualization tool OVITO was used for all the visualizations [28].

The intermolecular interaction between glycerol and diols have been first simulated, and the setup is shown in Figure 2(a). A number of glycerol and diol molecules have been randomly mixed, and then the box was relaxed at 300 K for 100 ps. Especially, for EG/glycerol=0.4, 13-PD/glycerol=0.4, and 12-PD/glycerol=0.4, the number of glycerol molecules was kept at 150, while the number of EG, 13-PD, and 12-PD molecules was 88, 72, and 72, respectively. To make a fair comparison, the total count of carbon atoms for EG/glycerol=0.6 was kept the same as the other systems, with the number of glycerol and EG molecules calculated to be 132 and 117, respectively. After 200 ps of relaxation, the intermolecular interaction between molecules has been analyzed.

The sliding simulation aims to reveal the distribution of lubricant molecules between the two sliding slabs during the sliding process. Figure 2(b) exhibits the configuration setup, two iron oxide (Fe_3O_4) slabs passivated with hydrogen atoms were employed as friction pairs, with each Fe_3O_4 slab dimension of $34.13 \text{ \AA} \times 34.14 \text{ \AA} \times 28.31 \text{ \AA}$. Each Fe_3O_4 slab consists of three parts: outer rigid layer, middle thermostatic layer, and inner non-thermostatic layer. The specific dimension could be seen in Figure 2(b). During the sliding simulation, 1 GPa pressure was applied to the top rigid top layer to push it downward approach the lower slab until the separation of the two slabs came to a relatively steady state. Then, the whole system was allowed to relax for another 100 ps, and the two thermostatic layers were coupled with 300 K. Finally, a shear velocity V_x of 10 m/s was applied to the top rigid layer, and the sliding motion lasted for another 800 ps. For the lubrication system of EG/glycerol=0.4, 13-PD/glycerol=0.4, and 12-

PD/glycerol, the number of glycerol molecules was kept at 100, and the number of EG, 13-PD, and 12-PD was 59, 48, and 48, respectively. As for EG/glycerol=0.6, the number of glycerol and EG molecules are 88 and 78, respectively.

The interaction between lubricant molecules with Fe_3O_4 surface was also analyzed. Figure 2(c) displays the configuration setup for this simulation process. Specifically, five lubricant molecules of glycerol, EG, 13-PD, and 12-PD were placed 5 Å beyond the iron oxide surface in a vacuum slab. The whole system was relaxed at 300 K and 1 atm for 100 ps, which was long enough to ensure the whole system reached the equilibrium state. Then, molecules were removed above this equilibrium state for a distance of 10 Å, far enough to neglect the interaction between the lubricant molecules and the Fe_3O_4 slab surface.

Through calculating the energy variation during this removal process, the adsorption strength could be obtained, which was useful to analyze the robustness of the adsorbed molecular layers and the related surface passivation ability.

3. Results

The friction performance of the prepared lubricant mixtures of EG/glycerol, 13-PD/glycerol, and 12-PD/glycerol with various diol/glycerol weight ratios has been evaluated at 4 N and 0.1 m/s on a ball-on-disk rotating tribometer at ambient atmosphere environment.

Figure 3 (a)-(c) displays the average COF evolution vs. the diol/glycerol weight ratio for the prepared diol/glycerol lubricant mixtures. For EG/glycerol lubrication system, as seen in Figure 3(a), superlow COF starts to appear from EG/glycerol=0.2, reaching the minimum of 0.005 at EG/glycerol=0.6. At EG/glycerol=0.8, COF increases above 0.01. 13-PD/glycerol accomplishes superlubricity at 13-PD/glycerol=0.4, as shown in Figure 2(b), with the minimum COF of 0.007. As seen in Figure 3(c), the average COF values for 12-PD/glycerol are all beyond the superlubricity regime, ranging from 0.013 to 0.018. Figure 3(d) illustrates some of the selected friction traces. Obviously, EG/glycerol=0.6 presents the lowest COF, with superlow friction achieved within 60 s. EG/glycerol=0.4 and 13-PD/glycerol=0.4 present similar friction traces, achieving superlubrication within 420 s. In the case of 12-PD/glycerol=0.4, about 1410 s is consumed before transiting to the vanishing friction state. Thus, it could conclude that the efficiency of these three diols in enabling superlubric behavior ranks in the following order: EG > 13-PD > 12-PD.

To further assess the wear performance, steel balls after the test have been cleaned to remove the residual lubricants and then analyzed under a microscope, as presented in Figure 4(a). Clearly, little surface damage is caused to steel balls with pure glycerol, EG/glycerol=0.4, and 13-PD/glycerol=0.6, with only some black deposits stacked around the wear area. Compared with EG/glycerol=0.4, EG/glycerol=0.6 sees slightly increased adhesive damage as well as increased formation of black deposits. Through Raman characterization of these deposits, as displayed in Figure 4(b), there are mainly two peaks at 1358 cm^{-1} and 1538 cm^{-1} that appear in the spectra, interpreted as lubricious oligomers [29-31]. It is not surprising that tribochemical reaction could be induced for glycerol and diols throughout the

sliding process, with similar results have already been reported in other literature studies [32-35]. It could expect that these in-situ formed oligomers could play a positive role by alleviating the asperity interaction across sliding surfaces.

As illustrated in Figure 3(a), EG/glycerol=0.6 exhibits superior superlubric behavior than EG/glycerol=0.4. However, Figure 4(a) shows that EG/glycerol=0.6 exhibits slightly increased wear damage than EG/glycerol=0.4. This contradictory phenomenon indicates the necessity of a specific investigation into the lubrication state of tribopairs. Figure 5(a) displays the viscosity of pure glycerol and diols. Pure glycerol presents an ultrahigh viscosity of 874 mPa·s, which is more than one order of magnitude than the three diols. As for diols, EG exhibits the lowest viscosity of 16 mPa·s, and 13-PD and 12-PD are similar with viscosity of about 48 mPa·s. Figure 5(b) presents the viscosity of the prepared diols/glycerol lubricant mixtures. Apparently, EG exhibits the highest viscosity reducing capability, followed by 13-PD, and finally 12-PD. A lower viscosity means reduced shear resistance within lubricant layers, desirable for reducing the energy dissipation caused by viscous flow.

Although less viscous lubricants are considered more fuel economy, it also risks bringing about more asperity contacts, causing high friction and wear. The theoretical minimum lubricant film thickness of the tribopairs has been evaluated via the widely used Hamrock–Dowson equation (as displayed in Appendix A1 [36, 37]). Figure 5(c) illustrates the plots of the calculated theoretical minimum lubricant film thickness. Apparently, the higher the diol/glycerol weight ratio is, the thinner the lubricant film is. At the same diol/glycerol weight ratio, EG/glycerol exhibits the lowest lubricant film thickness, next is 13-PD/glycerol, and the last is 12-PD/glycerol. Lambda ratio has been further calculated to evaluate the magnitude of asperity contact situation, and tribopairs with lambda ratio below 1 is believed to be in mixed/boundary lubrication state where relatively severe asperity interaction exists. As shown in Figure 5(d), lambda ratio drops below 1 for EG/glycerol at EG/glycerol = 0.4, while it is 13-PD/glycerol=0.8 for 13-PD/glycerol. In the case of 12-PD/glycerol lubrication systems, the lambda ratios are always beyond 1. Thus, the increased wear damage for EG/glycerol=0.6 should result from the intensified asperity contact between opposite surfaces due to the film decrease.

Limited load-bearing capability is a big concern for the future industrial application of macroscale liquid superlubricity. Here, we have explored the tribological performances of EG/glycerol=0.4, EG/glycerol=0.6, 13-PD/glycerol=0.4, and 12-PD/glycerol=0.4 at high loads of 5-7 N, and the results are presented in Figure 6. It is clear that EG/glycerol=0.4, EG/glycerol=0.6, and 13-PD/glycerol=0.4 always present reduced COF than pure glycerol, while 12-PD/glycerol=0.4 does not see any friction improvement. Figure 6(d) displays the calculated average COF at various loads. The maximum load is 6 N with the corresponding contact pressure of 827.84 MPa for EG/glycerol=0.4 and 0.6 to preserve the desirable superlow friction, while it is 5 N with the contact pressure of 779.03 MPa for 13-PD/glycerol=0.4 to maintain superlubrication. At the highest testing load of 7 N with the corresponding contact pressure of 871.49 MPa, the average COFs for EG/glycerol=0.4 and EG/glycerol=0.6 are still as low as 0.012, slightly above 0.01.

It is natural to think that what makes these diols with similar structures behave so differently? Considering the abundant hydroxyl groups these alcohol lubricant molecules have, it could anticipate that this difference could arise from the hydrogen-bonding (H-bonding) interaction. It has been reported that the ultrahigh viscosity of glycerol is due to its strong intermolecular H-bonding interaction that forms a three-dimensional hydrogen-bonding network [38]. Diols are miscible with glycerol since they could easily form intermolecular H-bonds with glycerol. The dissolved diol molecules could embed in the self-associated three-dimensional structure of glycerol molecules, as depicted in Figure 7(a), working as structure breaker to hinder the strong glycerol-glycerol interaction [39]. Due to the weakened glycerol-glycerol interaction, the diol/glycerol mixtures exhibit lower viscosity. The working efficiency of diol in modifying the rheological property of glycerol is related to its H-bonding interaction capability.

To analyze the intermolecular interaction of lubricant molecules, MD models has been established by mixing a certain number of glycerol and diols molecules and then relaxing the whole system for enough time. The number of intermolecular H-bonding for glycerol-glycerol and diol-glycerol have been counted, as displayed in Figure 7(b) and (c). Overall, EG could reduce the glycerol-glycerol intermolecular H-bonds more efficiently than 13-PD and 12-PD, and EG/glycerol=0.6 with a higher EG/glycerol weight ratio is more efficient than EG/glycerol=0.4. As for the diol-glycerol intermolecular interaction ability, EG/glycerol=0.6 and EG/glycerol=0.4 are on the first two places on the rank, followed by 13-PD/glycerol=0.4, with 12-PD/glycerol=0.4 ranked last. The superior intermolecular H-bonding capability of EG to 13-PD and 12-PD should be due to its lower molecular weight (62.07 g/mol), meaning that there are more EG molecules available to interact with glycerol than 13-PD and 12-PD (76.09 g/mol) at the same diol/glycerol weight ratio. Comparing the molecular structure of two propanediol, the two hydroxyl groups of 13-PD are located at the carbon chain ends, which are more exposed for intermolecular interaction than the hydroxyl groups of 12-PD molecules, which display a vicinal configuration [40-42]. In conclusion, EG exhibits the highest rheology modifying ability for glycerol due to its best intermolecular H-bonding interaction capability, followed by 13-PD, and 12-PD ranks last.

For a lubricant mixture, its friction performance is also affected by the distribution uniformity of lubricant molecules. MD sliding simulation has been carried out to help understand how the lubricant molecules distribute across the interface during the sliding test, and the results are illustrated in Figure 8. For EG/glycerol=0.4 and EG/glycerol=0.6, as seen in Figure 8(a) and (b), there are more EG molecules occurred near the sliding surfaces than that in the middle area. In the case of 13-PD/glycerol=0.6, as shown in Figure 8(c), 13-PD molecules tend to gather around the upper slab. In contrast, as seen in Figure 8(d), lubricant molecules of 12-PD/glycerol=0.4 present an even distribution. The enrichment of diol molecules near the sliding surfaces for EG/glycerol and 13-PD/glycerol could reduce the viscous drag of lubricant films to friction surfaces, beneficial to facilitating the relative sliding and reducing the shear resistance. In the meanwhile, the remaining part with reduced diol molecules would be slightly more viscous to better keep tribopairs apart [43]. Thus, such desirable distribution of lubricant molecules observed for EG/glycerol and 13-PD/glycerol is helpful to facilitate the relative sliding of tribopairs and reduce the sliding resistance.

Asperity interaction is always regarded as the main cause of high COF and wear. In our work, lubricant molecules of glycerol and diols abundant with hydroxyl groups have been employed, capable of adsorbing to steel surface to alleviate the severity of steel-to-steel interaction. As discussed before, though EG/glycerol=0.6 presents increased surface damage due to the lower lubricant film thickness generated, it still displays lower COF than EG/glycerol=0.4, confirming the formation of the protective adsorbed molecular layers. The specific interaction strength of lubricant molecules with iron oxide surface has been evaluated by MD simulation, with the results shown in Figure 9(a). Evidently, glycerol with three hydroxyl groups exhibits the highest average adsorption strength of 93 KJ/mol. As for three diols, the adsorption strength of EG (~67 KJ/mol) and 13-PD (~64 KJ/mol) is kind of higher than that for 12-PD (~62 KJ/mol). Figure 9 (b) - (e) illustrates the specific orientation of molecules on the iron oxide surface, and it can be seen that glycerol, EG, and 13-PD could always interact with iron oxide surface via their exposed hydroxyl groups, either in a flat or inclined direction. However, 12-PD could possibly attach to substrate surfaces using its methyl group, which is unstable and can be easily removed under shear. Thus, among the three diols, EG and 13-PD are more desirable than 12-PD for creating robust molecular layers to alleviate the steel-to-steel interaction. It could also anticipate that the lower molecular weight of EG could endow it with enhanced molecular layer-forming ability.

In conclusion, EG and 13-PD could provide robust superlubricity for steel tribopairs, while 12-PD with hydroxyl groups in a vicinal configuration is ineffective for this purpose. The difference arises mainly from two causes: one is their intermolecular H-bonding capability with glycerol molecules, and the other is the interaction ability with steel surfaces. The intermolecular H-bonding capability shows how efficiently that diols could break the strong self-association network of glycerol molecules, hence modifying the rheological property of the lubricant and making it less viscous. The interaction ability of lubricant molecules with substrate surface is related to the robustness of molecular layers formed on friction surfaces and its effectiveness in passivating steel-to-steel interaction without being sheared off easily. Compared with 12-PD, the hydroxyl groups of EG and 13-PD are more exposed that exhibit enhanced intermolecular H-bonding effect and higher interaction capability with steel surfaces. Furthermore, the MD sliding simulation also indicates that EG and 13-PD are prone to residing near the friction surfaces, beneficial to reducing the friction drag and facilitating the relative sliding. The lower molecular weight of EG molecules to propanediol makes it more competitive in preparing lubricants with superlubricity performance.

4. Conclusions

In summary, vanishing friction, *viz.* superlubricity state, has been enabled by mixing EG and 13-PD with glycerol, whereas 12-PD is ineffective for this purpose. Experiments and molecular dynamics simulations have been conducted to interpret the mystery. Some major conclusions are listed below:

(1) Diols could embed in the self-associated three-dimensional structure of glycerol molecules by intermolecular H-bonding interaction, working as structure breaker to hinder the strong glycerol-glycerol interaction, which hence makes the lubricant mixture less viscous and much easier to shear;

(2) Among three diols, EG and 13-PD with hydroxyl groups more exposed exhibit enhanced intermolecular H-bonding interaction than 12-PD with hydroxyl groups in a vicinal configuration; Owing to the lower molecular weight, EG is more desirable than 13-PD in preparing diol/glycerol lubricant mixtures with superlubricity performance;

(3) Sliding simulation shows that there are more EG and 13-PD molecules appear near the sliding surfaces, reducing the viscous drag to the sliding surface; while the remaining part with fewer diol molecules would be more viscous to separate tribopairs, beneficial to superlubricity achievement. Comparatively, 12-PD presents a uniform distribution;

(4) The more exposed configuration of hydroxyl groups for EG and 13-PD molecules could enable them to interact with steel surfaces with their hydroxyl groups, forming robust adsorbed lubricant molecular layers. 12-PD, with vicinal hydroxyl groups, could form weak and unstable adsorption points that could be easily removed by shear.

Declarations

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Figures

Glycerol

Glycerol

EG (Ethylene glycol)

13-PD (1,3-propanediol)

12-PD (1,2-propanediol)

Figure 1

Atomic structure of glycerol and diol molecules employed in this work.

Figure 2

(a) The intermolecular hydrogen-bonding interaction model for lubricant mixtures; (b) Computation setup configuration for sliding simulation, with EG/glycerol=0.4 was displayed here as an example; (c) Interaction analysis model for pure lubricant molecules with Fe₃O₄ surface, where the number of lubricant molecules was kept at 5 to minimize the intramolecular interaction effect.

Figure 3

Average COF for (a) EG/glycerol, (b) 13-PD/glycerol, and (c) 12-PD/glycerol lubrication systems with various diol/glycerol weight ratios. The average COF depicted here was calculated by averaging the whole friction curve except the initial 5 min to minimize the initial transient effect. (d) Friction curve vs. time for several selected lubricant mixtures.

Figure 4

(a) Optical micrographs of steel ball after the friction tests at 4 N and 0.1 m/s in pure glycerol, EG/glycerol=0.4, EG/glycerol=0.6, and 13-PD/glycerol=0.4; (b) Raman spectroscopy of deposits at the trailing edge of steel ball lubricated for pure glycerol, EG/glycerol=0.4, and 13-PD/glycerol=0.4.

Figure 5

(a) Viscosity of pure glycerol, EG, 13-PD, and 12-PD; (b) Viscosity of the prepared diols/glycerol lubrication systems versus diol/glycerol weight ratio; (c) Calculated theoretical minimum lubricant film thickness and (d) the corresponding lambda ratio. The viscosity presented were measured at 25 °C.

Figure 6

Friction performance of the selected lubricant mixtures (pure glycerol, EG/glycerol=0.4, EG/glycerol=0.6, 13-PD/glycerol=0.4, and 12-PD/glycerol=0.4) at various loads: (a) 5 N, (b) 6 N, and (c) 7 N. (d) Corresponding average COF evolution with the applied load. The average COF depicted here was calculated by averaging the whole friction curve except the initial 5 min to minimize the initial transient effect.

Figure 7

(a) Schematic illustration of the intermolecular H-bonding interaction between glycerol and EG; The number of intermolecular hydrogen-bonds (H-bonds) formed (b) between glycerol and glycerol and (c) between glycerol and diol for EG/glycerol=0.4, EG/glycerol=0.6, 13-PD/glycerol=0.4, and 12-PD/glycerol=0.4.

Figure 8

The number count of lubricant molecules between two iron oxide surfaces after 800 ps of sliding simulation: (a) EG/glycerol=0.4, (b) EG/glycerol=0.6, (c) 13-PD/glycerol=0.4 and (d) 12-PD/glycerol=0.4.

Figure 9

(a) Adsorption strength calculation of pure glycerol, EG, 13-PD, and 12-PD with iron oxide surface. The orientation of specific alcohol lubricant molecules on substrate surface: (b) glycerol, (c) EG, (d) 13-PD, and (e) 12-PD.