Effect of SiO₂ Particles on Thermo-Chemical/Mechanical Contact Behavior of PFPE Lubricants on DLC

Chang-Dong Yeo^{1)*} and Shahriar Mufid Rahman¹⁾

¹⁾Department of Mechaical Engineering, Texas Tech University, Texas, USA *Corresponding author: changdong.yeo@ttu.edu

The effects of SiO₂ contaminants on the airshear properties, friction force, and material transfer of PFPE lubricants were investigated through the molecular dynamics (MD) simulations with ReaxFF force field-based potential. The simulation results showed that the higher temperature, the more SiO₂ adsorption into the lubricants. The adsorbed SiO₂ particles increased the stiffness of PFPE lubricants leading to less airshear displacement. The adsorbed SiO₂ particles penetrated deeper into the Z-Tetraol than ZTMD lubricants. Also, the adsorbed SiO₂ particles caused to increase the magnitude of friction and the amount of lubricant pick-up during the sliding contact with a nanosized DLC tip.

Keywords: PFPE lubricant, SiO₂ contaminant, Airshear, Friction, Lubricant pick-up

1. Introduction

Due to the rapid heating by laser during heat-assistedmagnetic-recording (HAMR) operation [1], lubricants become thicker and more mobile, which accordingly can be evaporated at an elevated temperature. Such thermokinetically agitated or degraded lube can cause lube depletion on disk surface or contamination on head surface during HDI interaction. In this study, the thermochemical/physical behaviors of PFPE lubricants (i.e., thermal degradation, air shear dynamic movement, and lube pick-up) are systematically investigated in relation to HDI temperature and lube designs through systematic MD simulations.

2. Methods

2.1. Material Preparations

Two different types of PFPE lubricants, i.e., Z-Tetraol and Ztetraol multidentate (ZTMD), are prepared on DLC film as shown in Fig. 1(a) and (b). The molecular weight (MW) of Z-Tetraol and ZTMD is set to 2480 g/mol and 2610 g/mol, respectively. The lubricant thickness at 300 K is 11.8 Å and 8.9 Å, respectively. Due to the more functional end groups in ZTMD, it has higher stiffness and density than ZTMD leading to smaller lubricant thickness. SiO₂ particles are placed above the lubricant surface and then the energy equilibration process is conducted to enable SiO₂ adsorption into the lubricant layer.

2.2. MD simulations

In order to compare the physical property (i.e., stiffness or viscosity) of lubricant, airshear simulation is conducted as shown in Fig. 1(c). Under the controlled shear force, the amount of shear displacement of lubricant is measured. Next, a nanosized cylindrical DLC tip is sliding over the lubricated disk to measure the friction force and the amount of lubricant picked-up as shown in Fig. 4(d). The MD simulations are run with two different temperatures, i.e., 300 K and 700 K. All simulation schemes are performed on both noncontaminated PFPE and SiO₂-contaminated PFPE lubricants to examine the effects of SiO₂ on the lubricity of PFPE lubricants.



Figure 1: Scheme of MD simulations. (a) molecular structure of Z-Tetraol; (b) molecular structure of ZTMD; (c) Airshear simulation; (d) Sliding contact simulation to measure the friction force and lubricant pick-up behavior.



Figure 2: MD simulation results. (a) friction force; (b) the amount of lubricant pick-up after the sliding contact.

3. Results and Discussion

From the simulation results, it was observed that the higher temperature, the more SiO₂ adsorption into the lubricants. The adsorbed SiO₂ particles increased the stiffness of PFPE lubricants leading to less airshear displacement. Since Z-Tetraol has higher mobility with lower viscosity than ZTMD, the adsorbed SiO₂ particles penetrated deeper into the Z-Tetraol lubricants. Accordingly, the effect of SiO₂ was more obvious to Z-Tetraol lubricants. In addition, the adsorbed SiO₂ particles caused to increase the magnitude of friction and the amount of lubricant pick-up during the sliding contact with a nanosized DLC tip.

4. References

 Kryder, M. H. et al., "Heat Assisted Magnetic Recording," Proceeding of IEEE, 96, 11, 2008, 1810-1835.