A MOLECULAR DYNAMICS STUDY ON THE STATIC AND DYNAMIC PROPERTIES OF LUBRICANT PFPE IN HARD DISK DRIVER

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ABSTRACT
The static and dynamic properties of lubricant PFPE are important for the service durability and reliability of the computer head-disk device. Thus molecular dynamic simulations based on a coarse-grained, bead-spring model are adopted to study those properties. On the one hand, we investigate the static properties and infer the structure of both nonpolar and polar PFPE films. For a nonpolar PFPE film, there is a layering structure in the surface layer. And for a polar PFPE film, besides layering structure, there is a bi-polymer structure in the bulk layer. On the other hand, we investigate the dynamic properties and find that for nonpolar PFPE film, a precursor film around one atomic diameter thickness develops according to layering structure; while for polar PFPE film, besides a precursor film, a much steeper and slower spreading shape appears according to bi-polymer structure.

1. INTRODUCTION
To further increase the hard-disk storage areal density, a lot of efforts have been made to reduce the head-disk space, which may lead to the increase of contact probability in head disk interface [1]. Good lubricant mobility can make the lubricant molecules reflow at the interval between the two adjacent contacts, which ensures the hard-disk device to perform more efficiently and durably. A lot of experiments indicate that those properties, such as the interaction between the wall and the beads and the functionality of the end beads play the most important role in the properties of lubricant mobility. In this paper, molecular dynamic simulation is adopted to study the solid wall effect and the functionality of end beads effect on statistic and dynamic properties of lubricant PFPE for a durable and reliable computer head-disk device design.

2. MODEL AND SIMULATION METHOD
A coarse-grained, bead-spring model is adopted here, which was introduced in reference 2 for the application in PFPE films simulation. There are 216 or 96 polymer chains and 6 beads per chain in the static system and 648 polymer chains in the dynamic system. Molecular dynamic simulation using the canonical ensemble is employed to investigate PFPE film spreading on a solid wall. The fifth-order predictor-corrector algorithm due to Gear is used to integrate Newton’s equations of motion with a time step of \( dt = 0.001 \tau \), where \( \tau = \sigma (m/\varepsilon)^{\theta} \). For the static system, Nose-Hoover chain thermostat is used to maintain the average temperature, while for the dynamic system, a modificatory Nose-Hoover chain thermostat [3] is adopted.

3. RESULTS
The static properties of PFPE films can be described by the radius of gyration, the bead density, the end bead density. The end bead density represents the end bead number within the unit height, which mainly reflects the effect imposed by the functionality of the end beads, as is shown in figure 1.
First, we consider the effect from the wall. The static structure of polymer can be understood by dividing the system into two regions, a surface layer where there is an ordinal structure due to the wall and a bulk layer where there is an out-of-order structure similar to structure in bulk liquid. According to figure 1, the end bead density in the surface layer...
represents apparent oscillation with the adjacent peaks gap to be one atomic diameter, as supports a phenomenon that PFPE molecules are stacked near the wall layer by layer like solid substance in the surface layer. Next, we consider the effect from the functionality of end beads. According to figure 1(b), there appear two obvious peaks respectively at \( z=2.0\sigma \) and \( z=5.0\sigma \) with a gap approximately to be 4-5\( R_g \) (\( \sigma \) is one atomic diameter and \( R_g \) is radius of gyration of PFPE molecules). And the gap of 4-5\( R_g \) shows that there may contain two layers of PFPE molecules between two layers of the end beads. So we infer that for polar PFPE film, besides the layering structure in the surface layer, there is a bi-polymer structure in the bulk layer that two adjacent layers of polar PFPE molecules attract with each other through end beads to form a layer of molecules.

Thus we give a sketch for the structure of polar PFPE molecules inferred by the above results, as is shown in figure 2.

![Figure 1](image1.png)

**Figure 1** distribution of the end bead density in the direction perpendicular to the wall

![Figure 2](image2.png)

**Figure 2** structure of polar PFPE molecules

The dynamic properties can be described by the self-diffusion coefficient and profiles of a PFPE film spreading. Figure 3 and figure 4 show a series of profiles of PFPE film spreading on a solid wall, where \( X \) is in the direction of spreading, \( Z \) is in the direction of film falling down and \( t \) is the computing step. For nonpolar PFPE film, PFPE molecules slip down from film border to form a cap structure on the wall and diffuse along the wall to form a precursor film with a layer thickness around one atomic diameter which accords with layering structure in the surface layer, as is shown in figure 3. For polar PFPE film, besides a precursor film, a much steeper and slower spreading shape appears according to bi-polymer structure, as is shown in figure 4. And we consider the phenomenon for polar PFPE film results from hydrogen bond interaction between end beads and end beads.

![Figure 3](image3.png)

**Figure 3** nonpolar PFPE film spreading on a solid wall

![Figure 4](image4.png)

**Figure 4** polar PFPE film spreading on a solid wall

### 4. CONCLUSION

Molecular dynamic simulation based on a coarse-grained, bead-spring model is adopted to investigate the static properties and the dynamic properties as a function of the wall effect and the functionality of PFPE films effect. We infer the structure of both nonpolar and polar PFPE films. And we consider the interaction between the wall and PFPE molecules as the main factor for development of a precursor film. At the same time, we point out that the functionality of the end beads may slow the film diffusion for the bi-polymer structure.

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### REFERENCES