

Molecular dynamics simulation for ultrathin lubricant nanofilms with nonfunctional and functional end groups

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Abstract

In this paper, the molecular conformation and end bead density profile of the lubricant nanofilm at head disk interface are examined via molecular dynamics simulations using coarse-grained, bead spring model. It is indicated that the PFPE chains have an oblate conformations near the wall, but gradually transform into spherically shaped, bulk configurations as the lubricants move away from the wall. The end group functionality does not have significant effect on the molecular conformation.

1. Introduction

In order to achieve a higher areal data density of hard disk drives, the flying height between the air bearing slider and the lubricant film is decreasing steadily, i.e., the flying height has to be reduced to less than 5 nm to gain an areal density of one Terabit per square inch [1]. Under such extremely small distance, the lubricants play an increasingly important role in the head disk interface (HDI) stability and reliability [2, 3]. The mostly commonly used lubricants in hard disk drives are perfluoropolyethers (PFPEs). Due to the difficulties and complexities of the experimental work, the static and dynamic properties of the lubricant nanofilms are not well studied at the nanometer scale. Therefore, a molecular level modeling and simulation of the ultrathin lubricant nanofilm at HDI has drawn great interest and concern [4-6]. In this paper, the molecular dynamics (MD) simulations with coarse-grained, bead spring models are adopted to investigate the molecular conformation and layering structure of PFPEs with nonfunctional and functional end groups.

2. Simulation model and methodology

The coarse-grained bead spring model, which simplifies the detailed atomic structure but still maintains the essence of the intermolecular interaction, is utilized to investigate the static and dynamic properties of PFPE lubricants.

Each polymer chain consists of a number of beads (N_p) that are connected by a nonlinear spring and the bead number is related to the molecular weight (MW). In our MD simulations, the number of beads per one chain is set to be 10, which approximately has MW of 2000 g/mol. By assigning beads with different functionalities, they can be categorized into backbone beads (*bb*) or end beads (*eb*) during the simulation. Moreover, the smooth disk surface that lies on the x - y plane is regarded as an infinitely long and infinitely deep flat surface, and is oriented at $z = 0$ to save the computation time.

The finitely extensible nonlinear elastic (FENE) potential is used to describe the neighboring beads as well as the end beads. To compute the interactions between the beads, and between the beads and the solid surface (wall), the 12-6 and 9-3 Lennard-Jones potentials are employed respectively. The interactions between the end beads and the wall, and the interactions between the end beads can be expressed using short-range exponential decay functions.

In our MD simulations, there are 300 PFPEs chains. The entire chain moves according to the Newton's second The velocities of the PFPEs chains are rescaled and a Verlet neighbor list is reconstructed at every 20 time steps. Periodic boundary conditions are applied in the x and y directions.

3. Results and discussion

The molecular conformation of the lubricants is examined via the anisotropic radius of gyration – in parallel and perpendicular components:

$$R_{\parallel}^2 = \frac{1}{2N_p} \sum_{i=1}^{N_p} \left[(x_i - x_g)^2 + (y_i - y_g)^2 \right] \quad (1)$$

$$R_{\perp}^2 = \frac{1}{N_p} \sum_{i=1}^{N_p} \left[(z_i - z_g)^2 \right], \quad (2)$$

In Eqs (1) and (2), N_p is the number of beads in one chain, (x_g, y_g, z_g) are the coordinates of the PFPE molecule's center of mass, and (x_i, y_i, z_i) are the coordinates of the beads.

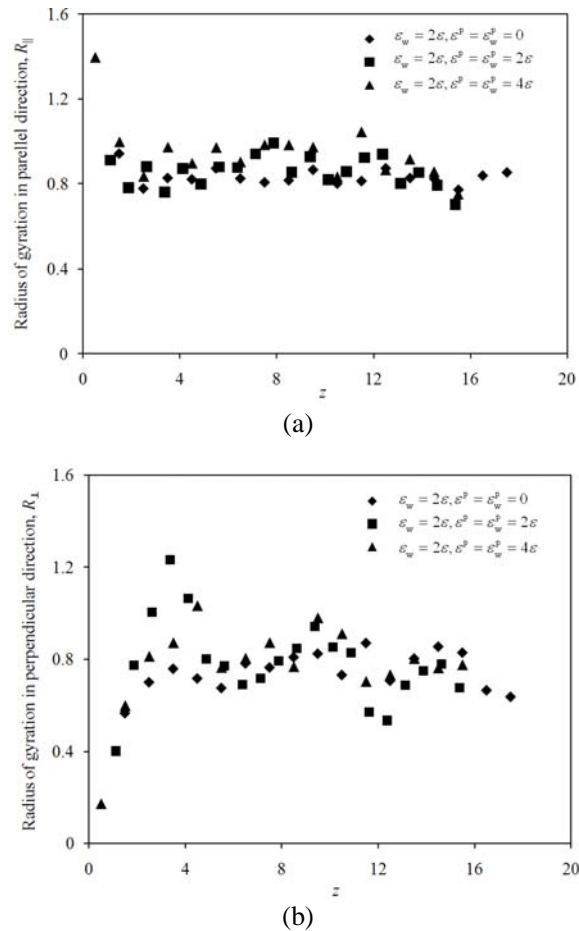


Fig. 2. Radius of gyration as a function of the distance from the wall z : (a) parallel component and (b) perpendicular component.

By calculating the radius of gyration as shown in Fig. 2, it is observed that the chain conformation becomes more oblate as the lubricant chain approaches the wall. However, it recovers its spherically shaped bulk configuration when it moves away from the wall. It is also notable that the functional end group does not significantly affect the radius of gyration.

4. Conclusion

The static property, such as molecular conformation, is examined via MD simulations using coarse-grained, bead spring model. The oblate conformations of the PFPE chains are transformed

into spherically shaped, bulk configurations as the lubricants move away from the wall. It is also observed that the film conformation depends weakly on the end group functionality.

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