PRESSURE IN ULTRA THIN PERFLUOROPOLYETHER FILM

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ABSTRACT

The density and pressure variations in the ultra thin liquid perfluoropolyether (PFPE) film (2nm) are carried out by Monte Carlo simulations of Lennard-Jones systems. First of all, the variations of density and pressure of ultra thin PFPE film that has a free surface on the flat substrate are carried out. The substrate is assumed to be continuous without atomic structure and exerting Lennard-Jones potential on liquid molecules in the ultra thin film. Next, the variations of density and pressure in the ultra thin PFPE liquid film between the two solids are examined. This is assumed to be due to the contact between the flying head and the PFPE film. From results of the 2500 steps calculation, it is clarified that the density distribution between two solids becomes symmetrical in shape and the pressure distributions concentrate on the substrate surface and the flying head surface do not occur in the liquid between the two surfaces.

1. INTRODUCTION

Recently, the recording density of magnetic disc storage devices has increased remarkably. In order to increase the recording density of the magnetic disc storage device, it is essential to decrease the mechanical spacing between the magnetic disc and flying head. As a result, the contact between the flying head and the lubricant on the disc surface is unavoidable. Hence, the lubricant has to be self-spreading. In order to satisfy these demands, it is necessary to clarify the fundamental characteristics of the ultra thin lubricant film.

Generally, PFPE is used as a lubricant of the magnetic storage discs. The film thickness is estimated to be about 1.0 to 2.0 nm and consists of mono to several molecular layers. Therefore, in order to clarify the phenomena of lubricant in the microscopic and nano-scale region, it is quite difficult to apply the traditional continuum theory to such a lubricant. There fore, it is necessary to understand the lubricant film characteristics under molecular structures.

In this report, simulation of a lubricant that has a free surface on the flat substrate (disc), and a lubricant sandwiched between the two flat solid surfaces (supposing that the flying head touches the lubricant) was carried out using the Monte Carlo simulations of Lennard-Jones systems. The simulations were done in terms of the variation of density and pressure generated in the ultra thin PFPE lubricant film.

2. Simulation model

2.1 Beads model

The chemical formula for the PFPE Z lubricant is [F-CF₂-OCF₂-CF₂]ₘ-OCF₂-F, n/m=2/3, and the molecular weight is 4000g/mol. Each polymer chain consists of a sequence of beads bonded by a potential energy and consisted of 16 beads. Molecular length of 4000g/mol is 14nm and the interval of beads is 0.933nm.

2.2 Calculation condition

As shown in Fig.1, a box type system is supposed as the existence region of beads, and the periodic boundary conditions as shown in Table 1 are adopted. In calculations, Monte Carlo simulations based on Lennard-Jones potential is used. Each calculation is repeated 10,000 steps. The results of the 2500 steps calculation are shown in Fig.2.

3. Density and pressure distribution of beads

Figure 2 shows the density distribution of PFPE film put freely on flat solid surface after 10,000 step calculations. This distribution is obtained from the number of beads that exist in...
the volume divided in every 0.1 nm layer in z direction [3]. It is seen that extremely large volume beads are distributed near the solid surface. It is considered that these are the adsorbed molecules.

![Coordinate system](image1.png)

**Table 1** Box length and Boundary conditions

<table>
<thead>
<tr>
<th>Box</th>
<th>Direction</th>
<th>Ultrathin films</th>
</tr>
</thead>
<tbody>
<tr>
<td>Box size</td>
<td>x and y</td>
<td>32/fD</td>
</tr>
<tr>
<td>Side BC</td>
<td>x and y</td>
<td>2 nm</td>
</tr>
<tr>
<td>Top BC</td>
<td>z</td>
<td>Periodic</td>
</tr>
<tr>
<td>Bottom BC</td>
<td>z</td>
<td>Solid surface</td>
</tr>
</tbody>
</table>

![Density variation in the ultrathin liquid film of PFPE on solid surface](image2.png)

Figure 2 shows the density variation in the ultrathin liquid film of PFPE on solid surface. Figure 3 shows the pressure distribution of the ultrathin liquid film of PFPE on solid surface at 10,000 MC steps.

![Pressure variation in the ultrathin liquid film of PFPE on solid surface](image3.png)

The calculations of density variation and the pressure distribution in the ultra thin film of PFPE were achieved in between the solid surfaces and the free end surface.

**REFERENCES**


![Density variation in the ultrathin liquid film of PFPE between solid surfaces (2500MC steps)](image4.png)

Figure 4 and 5 shows the density and pressure distribution of PFPE film sandwiched by two solid surfaces after 2500 step calculations, respectively. It is seen that the distributions of density and pressure show a symmetrical pattern. This depends on the adsorption phenomena to the upper surface (flying head) that is touching the liquid film.

![Pressure variation in the ultrathin liquid film of PFPE between solid surfaces (2500MC steps)](image5.png)

**4. Conclusion**

The calculations of density variation and the pressure distribution in the ultra thin film of PFPE were achieved in between the solid surfaces and the free end surface.