SOME ASPECTS OF THE NANOLUBRICANT FILM IN NANOTRIBOLOGICAL APPLICATIONS

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Abstract: *During the last decades requirements in engineering are continuously increasing, and as a consequence of this, nanolubrication regime experienced a remarkable development. In this respect, molecular dynamic simulations were used to characterize changes in lubricant properties that occur during nano-elastohidrodynamic lubrication. In this context, our attention is focused on confined nanofilms, the simulations being supported at variable speeds wall and different loads.*

Keywords: *nanotribology, nanolubrication, molecular dynamic simulations*

1. Introduction

The word tribology is not a very old word, coined in 1966, but its application was done since Paleolitic period. To reduce friction was a task BC in order to transport large stone building blocks, using water-lubricated sleds. Although the viscous flow laws have been postulated by Newton, scientific understanding of lubricated operations appears at the end of 19th century. Since then, the development of experimental and theoretical techniques has growing. In the 20th century the industry "ask" for a better tribology, leading to an expansion of our knowledge of it. The researchers in tribology are now forced to eliminate the losses resulting from friction and wear at all levels of technology. And this is not an easy task.

In this respect, in our days we are talking about nanotribology, encountered in magnetic storage systems, MEMS/NEMS and other industrial applications. The nanotribological studies are important in order to understand the phenomena at the atomic scale, let's say been a bridge between physics and engineering [1, 2]. Consequently, the computational physics or chemistry has been used since the early 90s.

Widely used in nanotribological studies was surface force apparatus (SFA), scanning tunneling microscope (STM), atomic-force and friction-force microscope (AFM and FFM). Meanwhile, the imposed progress has lead to a better understanding of atomic-scale energetic, structure thermodynamics and rheological aspects of tribological process. Today, the lubrication by thin films is a remarkable research topic, the lubricant film thicknesses continuously decreasing, becoming the order of a few nanometers. At this level, the conventional laws are unable to explain the encountered phenomena. In this respect, investigating also the molecular effects, the molecular dynamics simulations has been proved to be an effective tool for a proper understanding of the phenomena [3-5].

If we turn to applications, the magnetic storage industry is a few hundreds of billions per year, while in data storage industry is around few billion per year. Magnetic recording involves the relative motion between a magnetic medium against a read-write magnetic head. Heads develop a hydrodynamic air film under steady operating conditions to minimize head-medium contact [6]. However, physical contact between them is going during starts and stops.

An important aspect in tribology is the type of lubricant. For example, in case of hard disk is must assure longer durability and disk-surface protection in case of slider-disk contact. The most commonly used disk lubricants are perfluoropolyethers (PFPE); they are sufficiently slippery, and provides good surface wetting properties. Also, PFPEs present shear stability and excellent lubricity under normal and severe conditions.

2. Simulation method

In the last decades, the field of nanolubrication recorded a remarkable scientific development. The lubricant film thicknesses decreasing and new and challenging initial conditions are involved, such as high load. Computer simulations performed by the researchers reveals a layered structure and a density profile for the lubricant film [4, 7, 8].

In this paper, our attention is focused on 3.5 nm lubricant films thickness, equivalent to 100 molecules, in regime of non-equilibrium molecular simulations (NEMD). The simulations were performed with Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [9]. The PFPE lubricant film is confined between gold walls, the force field being AMBER (figure 1).

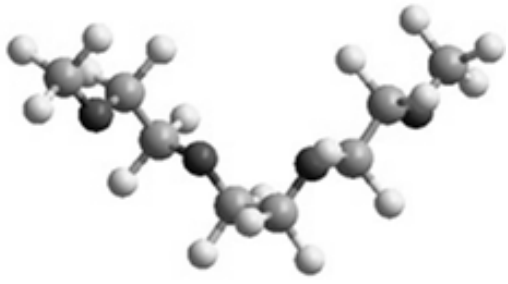

Figure 1: *The molecular model of PFPE-Z ($C_8F_{18}O_4$). Carbon atoms are gray, fluorine is white, and oxygen atoms are black.*

For a proper analysis we are considering the stretching of bonds, the torsion angles and van der Waals potential, so in our simulations we need of van der Waals, bond, torsion, and angle parameters, along with electric charges. The full simulation method is described in one previous paper [10].

In this work we investigate the case when only the upper wall is moved at constant velocity (figure 2), and when both walls are moving in opposite directions for several investigated velocities (figure 3). To analyze the load effect, the upper wall is supporting different constant load.

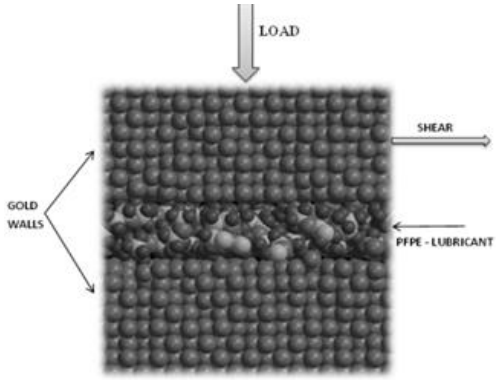

Figure 2: *Snapshot of the simulation cell*

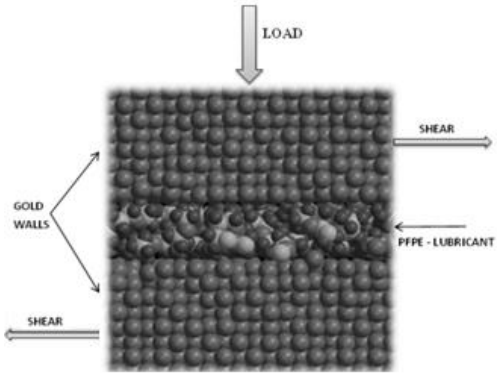

Figure 3: *Snapshot of the simulation cell*

3. Results

In the figure 4 we represented the velocity profile in the case of high load, when the bottom wall is at rest. We may notice a strong slip at both walls; it is like the lubricant film is moving with a lower speed than the upper wall (figure 4). Looking at the density profile we can observe a stratification of the film, film which is confined between the walls (figure 5).

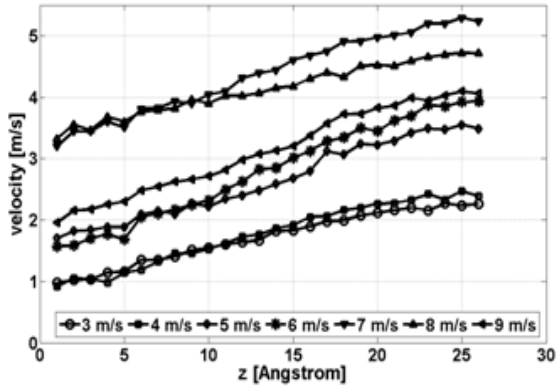

Figure 4: *The velocity profile at different sliding velocities, for 1.5 GPa load*

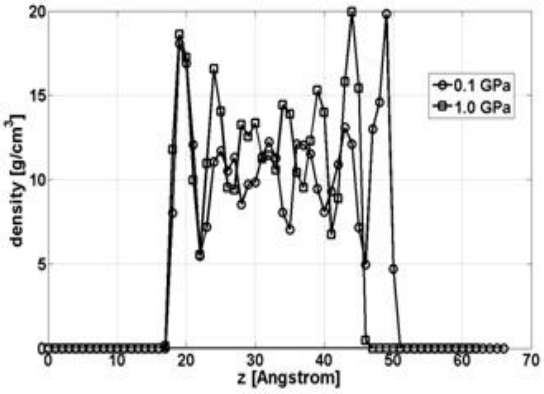

Figure 5: *The density profile for v=6 m/s*

In figure 6 we analyze the velocity profile at different loads, for 6 m/s sliding velocity, when both walls are moving in opposite direction. We may see that at low load (0.1 and 0.5 GPa) a stick is revealed at the bottom wall, the lubricant near the wall having around 4 to 5 Å. Except for this stick, the lubricant film shows a Newtonian behavior.

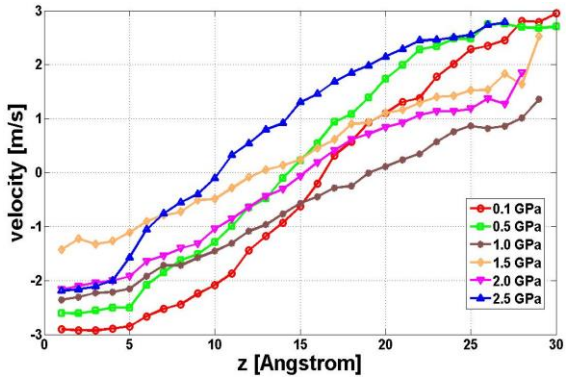

Figure 6: *The velocity profile at different loads, v=6 m/s*

Increasing the load at 1.0 GPa we encountered slip at both wall, while at 1.5 GPa the slip is at the bottom wall.

Examining the radial distribution function at the beginning of the experiment the lubricant film is fluid (figure 7), while at the end of it the lubricant film became like a solid, confirmed by the appearance of the second peak.

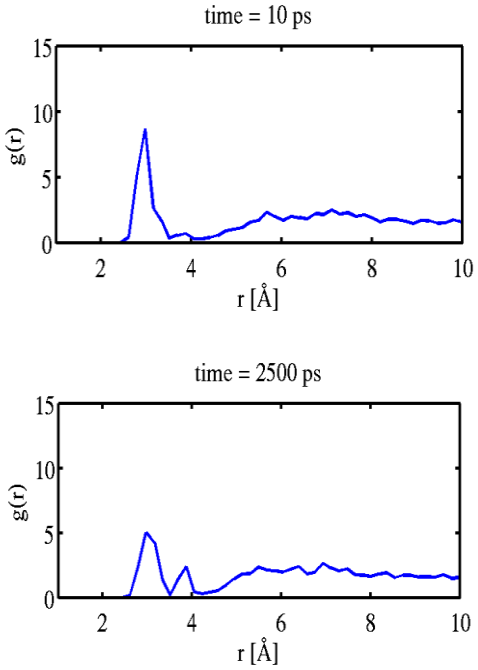

Figure 7: *Radial function distribution for 1.5 GPa load and v=6 m/s*

Another important aspect of characterizing the lubricant behavior is related to the friction force. In the next two figures we represented the friction force when both sliders are moving.

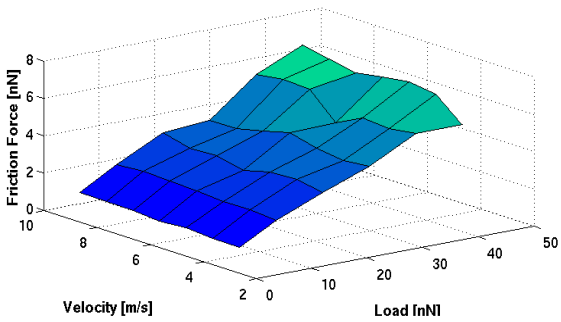

Figure 8: *The friction force as a function of velocity and load*

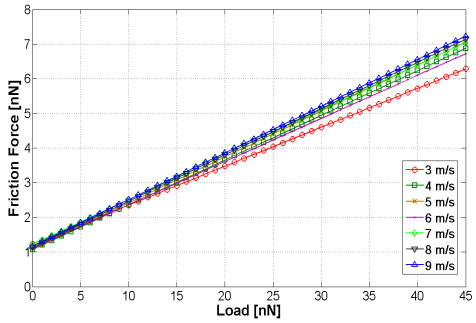

Figure 9: *The friction force as a function of load*

Looking at the figure 9 we see that the friction coefficient slightly depends on the walls speed. We suppose that this dependence is due to interactions between lubricant molecules and the interactions between them and the walls.

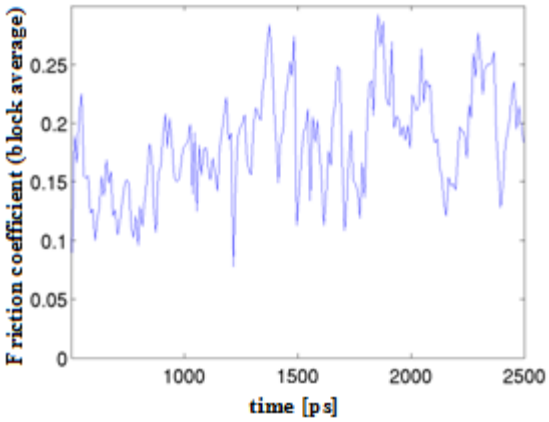

Figure 10: *The friction coefficient as a function of time*

The friction coefficient changes periodically (figure 10). We are able to say that when the friction coefficient increase, the lubricant film is distorted, which happens when the lubricant molecules stick to the wall. On the other hand when this coefficient decreases, practically the slip phenomena are involved. When stiction force to the wall is lower than friction force, the slip is present, then, friction decrease and the lubricant film is in initial state. Therefore, this slip and stick cycle may cause this friction coefficient changes.

Conclusions

In this article, we investigated the confined lubricant film (PFPE) behavior, using NEMD.

The thickness of the film is 3.5 nm meaning 100 molecules. Our results were obtained investigating the case when only the upper wall is moving, and both walls are moving in opposite direction. We may notice that the lubricant is layered, the slip-stick phenomena being present for different conditions. The last ends are strengthened by friction coefficient changes.

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