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ALL-ATOM MOLECULAR DYNAMICS SIMULATION OF SUBMICRON THICKNESS EHL OIL FILM

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ABSTRACT

All-atom molecular dynamics simulations of an elastohydrodynamic lubricating oil film have been performed to study the effect of the oil film thickness (large spatial scale; thickness: 430 nm, MD time: 25 ns) and the effect of pressure (long time scale; thickness: 10 nm, MD time: 50 ns, external pressure: 0.1 to 8.0 GPa). Fluid layers of *n*-hexane are confined between two solid Fe plates by a constant normal force. Traction simulations are performed by applying a relative sliding motion to the Fe plates. In a long spatial scale simulation, the mean traction coefficient was 0.03, which is comparable to the experimental value of 0.02. In a long time scale simulation, a transition of the traction behavior is observed around 0.5 GPa to 1.0 GPa which corresponds to a change from the viscoelastic region to the plastic-elastic region which have been experimentally observed. This phase transition is related to a suppressed fluctuation of the molecular motion.

INTRODUCTION

Machine elements in which large loads are transmitted such as a traction drive continuously variable transmission (CVT) work in the elastohydrodynamic lubrication (EHL) regime. The molecular dynamic behavior of the oil film under EHL is not well understood, since long trajectories of a ensembles of large number of fluid molecules are required to analyze the drastic phase transition induced by high pressure [1-4]. A typical practical EHL condition includes a film thickness of submicron order and a shear rate less than 10^6 /s. Although this film thickness exceeds the range of the van der Waals structural force of the solid plates, the behavior of the fluid layer differs from the bulk, i.e., the traction coefficients (the tangential traction force divided by the normal load) cannot be easily deduced from the bulk shear viscosity. In this study, a molecular dynamics (MD) simulation on a shared-memory parallel computer was used to study the effect of the oil film thickness and the effect of pressure.

METHOD

Fluid layers of *n*-hexane are confined between two solid α-Fe crystal plates under a constant normal force (external pressure p_{zz}). Traction simulations are performed by applying a relative sliding motion to the Fe plates. The traction coefficients μ were calculated from the horizontal stress on the Fe walls. The fluid molecules are dynamically treated using the AMBER force field. The temperature is controlled at 350K using Nosè-Höver formalism. The details are shown in ref. [1-3].

The solver was parallelized by a Message Passing Interface (MPI), and the MD runs were done using up to 24 nodes (384 processor).

LARGE SPATIAL SCALE SIMULATION

In our previous simulation of a thin film thickness z_0 of 1 - 10 and the high shear rate of 10^7 -10^9 /s, our calculated traction coefficients showed higher values than the experimental ones over the entire simulation range [1]. The simulation of an oil film with a realistic thickness of 430 nm (Fig. 1) yields a mean traction coefficient of 0.03, which is comparable to its experimental value of 0.02 [1, 3]. According to the density profiles (Fig. 2), although no remarkable layered structure originating by the oscillating wall force shown in the vicinity of the boundary is found in the center, a small oscillation corresponding to the thickness of the molecular

layers remains, which suggests the effect of the shear field, reaches the center of the oil film.

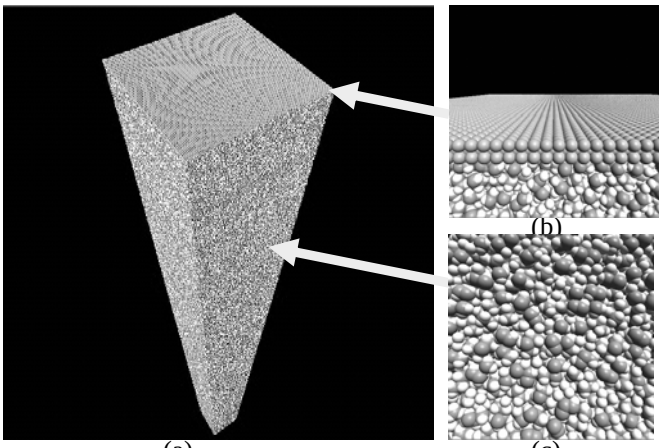


Fig. 1 Snapshots of the molecular dynamics simulation of submicron (430nm) thickness oil layer (a). In the vicinity of solid atom plate (b), Center of the film (c). External pressure $p_{zz} = 1.0$ GPa, relative sliding speed = 0.1 m/s.

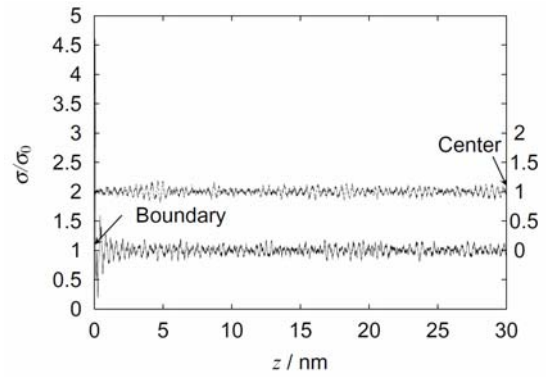
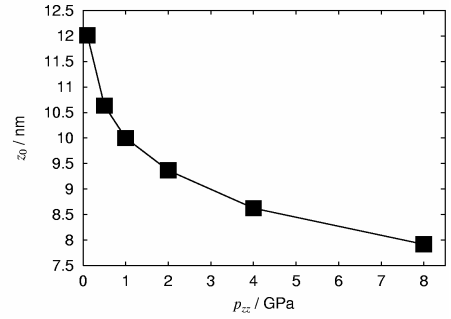


Fig. 2 Density profiles of carbon atoms obtained from simulation of film thickness of 430 nm. 30nm in the center and boundary of the oil film are shown.

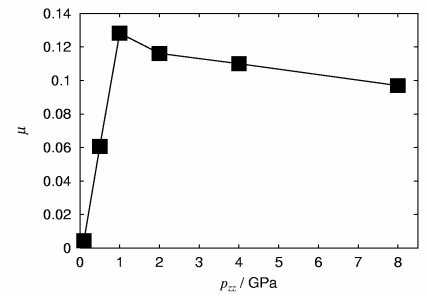
LARGE TIME SCALE SIMULATION

The effect of the external pressure p_{zz} was studied by the long time scale simulations of 50 ns in each p_{zz}. The number of molecules are fixed to 576 that corresponds to the film thickness of $z_0 = 10$ nm at $p_{zz} = 1.0$ GPa. The limiting shear stress transition of the traction coefficients is observed around from 0.5 GPa to 1.0 GPa (Fig. 3) that corresponds to the phase transition from the viscoelastic region to the plastic-elastic region which is experimentally known [5].

The molecular mechanisms of the phase transition are analyzed by the radial distribution functions and the velocity profiles. In the radial distribution functions (Fig. 4), liquid-like distributions, which have a single peak, are found at the low pressure of 0.1 to 0.5 GPa. As the pressure increases, the sharpness of the peaks increases and a shift in the peaks are found, whereas the obvious transition of the curves around 1.0 GPa is not found. This means that the transition is not related to



(a) Film thickness.



(b) Traction coefficients.

Fig. 3 External pressure dependence on film thickness and traction coefficients calculated from long timescale simulation. *n*-Hexane: 576 molecules, Sliding velocity: 1 m/s.

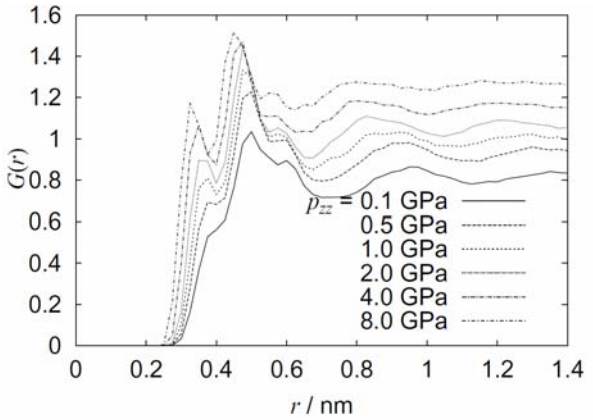


Fig. 4 Radial distribution functions of carbon atoms $G(r)$ at various external pressures. The intramolecular atoms are not shown. All lines are normalized by average concentration at p_{zz} = 1.0 GPa.

only the arrangement of the molecules.

In order to discuss the motion of the molecules, the velocity profiles at low pressure (p_{zz} = 0.5 GPa) and at high pressure (p_{zz} = 2.0 GPa) are plotted in Fig. 5. The Newtonian-like profiles are shown at low pressure, whereas the non-Newtonianity becomes stronger at the high pressure which suggests an increase in the elastic interactions of the molecules. The difference in the molecular motion at high and low pressures are clearly shown in the profiles of the velocity fluctuation (Fig. 6). At a low pressure, the degrees of fluctuation in the velocity are greater than at a high pressure and the plateau region is found in the center of the oil film. At a high pressure, the plateau region is not found which indicates that the effect of the wall reaches to the center of the film. This suggests that the plasticity is related to the suppression of the molecular motion fluctuations.

CONCLUSIONS

A quantitative agreement of traction coefficient between experiment and molecular dynamics simulation is found by simulating the oil film with a realistic thickness of submicron order.

The limiting shear stress of the EHL molecular oil film is reproduced by the simulation. This phase transition is related to the suppression of the molecular motion fluctuation.

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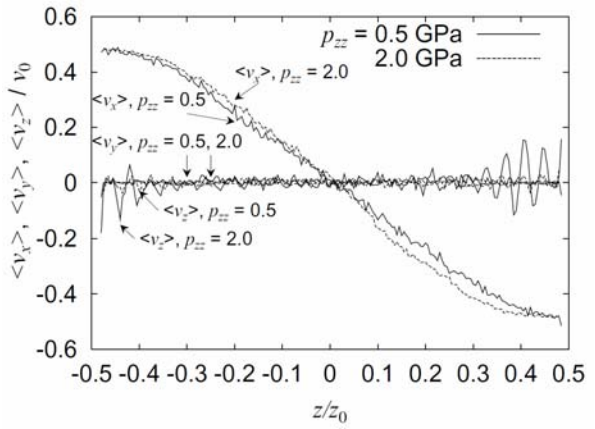

Fig. 5 Velocity profiles at low pressure (solid line, p_{zz} = 0.5 GPa) and at high pressure (dotted line, p_{zz} = 2.0 GPa). *x*: sliding direction, *y*: transverse direction, *z*: film thickness direction.

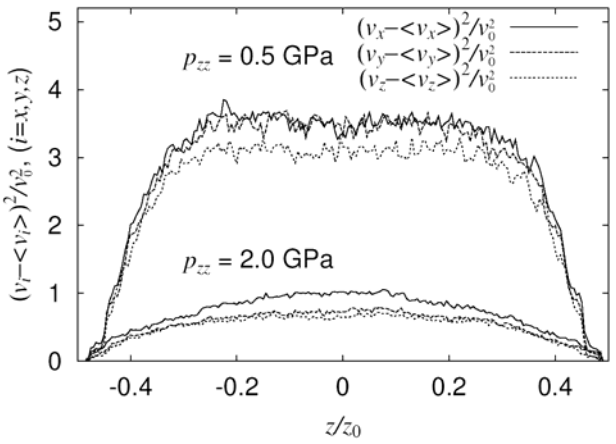

Fig. 6 Profiles of velocity fluctuation at low pressure (lower curves, p_{zz} = 0.5 GPa) and at high pressure (upper curves, p_{zz} = 2.0 GPa). The notation of *x, y, z* are same as Fig. 5.