Molecular Dynamics Simulation and Structural Analysis of Traction Fluid

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Traction mechanism in shear field and high pressure for several kind of fluids are studied by molecular dynamics. The traction coefficient of two kind of molecules, alicyclic dumbbell compounds $C_{18}H_{30}$ and long chain alkane poly(1-ethylethylence)$_{15}$, in various conditions to find important factor for traction. The calculated traction coefficient decreases with temperature rise same as experiment. The mechanism of temperature dependence is then analyzed for each molecule.

Keywords: Elasto-hydrodynamic lubrication, molecular dynamics, traction fluid

1. Introduction

Traction drive is a machine that transmits power by a rotor and lubricating oil called traction fluid. Traction fluid is required high traction coefficient to propagate the force efficiently, however, the mechanism of traction force has not been sufficiently elucidated, since the phenomena occur in elasto-hydrodynamic lubrication region. In this paper we evaluate the characteristics of the fluid molecules in the traction drive using molecular dynamics and experiments, both for long chain molecules which is used for stationary system such as elevator, and alicyclic dumbbell compounds for automotive transmission.

2. Methods

In this simulation, the system consists of traction fluid and solid walls [1-3]. Two types of traction fluid are simulated. One is poly(1-ethylethylence)$_{15}$, and the other is alicyclic dumbbell compounds $C_{18}H_{30}$. Solid walls are imitating (100) surface of α-iron, and their atomic motion is frozen. First, a pressure is applied in the z direction. Constant sliding velocities in opposite direction are then applied to the walls. The interaction of the solid and fluid is enhanced to suppress the slip at interface [1,2]. Then, the simulation time on the order of nanoseconds is passed and the steady state is set. The Simulations using LAMMPS are calculated at various conditions (Table 1). Generalized amber force field is used to calculate the interactions for organic molecules.

Table 1: parameter settings

pressure [GPa]	0.8-1.24
sliding speed [m/s]	0.5-100
temperature [K]	253-413
time step [fs]	0.5
boundary condition	X, Y: periodic Z: fixed

3. Results and discussion

Since the calculation for the long chain molecules are the first time, we evaluated the reliability of the simulation method by changing the size of solid layer and sliding conditions. The validity of the method is confirmed for the number of monomer of poly(1-ethylethylence) N_{mono} up to 30. Figure 1 (a) shows temperature dependency of Traction coefficient of poly(1-ethylethylence)$_{15}$, which decrease with temperature rise, same as experimental result. Figure 1 (b) shows the distribution of the dihedral angles at the center of dumbbell structure of $C_{18}H_{30}$. It is found that there are three stable structures.

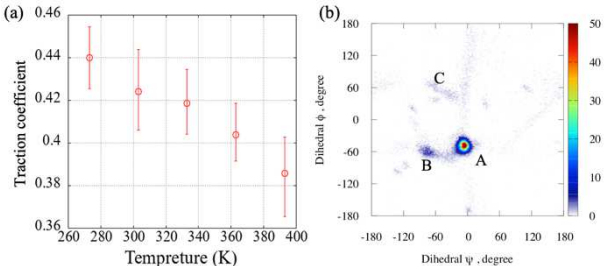

Figure 1: (a) Temperature dependence of traction coefficient of poly(1-ethylethylence)$_{15}$ (N_{mono}=15), (b) Distribution of dihedral angles of $C_{18}H_{30}$.

We calculated with another degree of polymerization, N_{mono}= 6 and 30. The traction coefficients are 0.342 (N_{mono}=6), 0.418 (N_{mono}=15), and 0.437 (N_{mono}=30), which increases as the degree of polymerization increase. For the long chain molecules, the degree of internal momentum transfer is not negligible. For the dumbbell like molecules, the distribution of dihedrals changes as the physical conditions, high-pressure and shear field. By time series analysis, it is confirmed that the transition between structure A and B, A and C is frequently. The difference of the molecular mechanism of momentum transfer is clarified.

4. References

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