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Review

Molecular Dynamics Analysis of Elastohydrodynamic Lubrication Oil Film

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■ABSTRACT■ This paper reviews the recent research regarding the non-equilibrium all-atom molecular dynamics studies of the traction properties of hydrocarbon fluids under elastohydrodynamic lubrication. The effect of the oil film thickness, shear rate and pressure were studied. The dynamic mechanisms of the momentum transfer on layers of fluid molecules are analyzed focusing on the intermolecular interactions and intramolecular interactions. Characteristic molecular mechanisms are obtained for the high traction molecules of cyclohexane and dumbbell-like molecules (dicyclohexyl, dicyclohexylmethyl and santotrac 50). In the dumbbell-like molecules, alicyclic rings, which distribute across the low ordered molecular layers, behave as a stiff bulky mass, and momentum transfers to the end of the molecular axis. The traction mechanisms of hydrocarbon fluids are also determined during the course of the analysis. The method would be applied to design composite fluid molecules of high-performance traction oil.

■KEYWORDS■ Molecular Dynamics, Traction Fluid, Elastohydrodynamic Lubrication, Hydrocarbon, Momentum Transfer

1. Introduction: Tribo Molecular Dynamics

In this paper, we briefly describe the history of molecular dynamics (MD) simulations applied to tribology, and introduce some examples of research regarding the analysis of molecular mechanisms of elastohydrodynamic oil films.

MD is a numerical simulation method in computational chemistry or physics which describes the motion of atoms under classical approximation by solving Newtonian equations of motion.⁽¹⁾ **Figure 1** shows the time development of a number of scientific articles, which contain the keyword “Tribology” or “Lubrication” and “Molecular dynamics” in the title or in the abstract, which are found in the Web of Science database by Thomson Reuters.

The MD studies which focus to “Tribology” or “Lubrication” started in the 1990s and made rapid progress in the late 1990s. We hereafter call these studies “Tribo Molecular Dynamics”.

Before the beginning of the Tribo MD, many studies corresponding to this topic have been done. The origin of the MD method can be traced back to a calculation of dynamics of hard sphere particles by Alder and Wainwright in the late 1950s.⁽²⁾ At the beginning,

subjects of the simulations were mainly the phase transitions of solids and liquids, then the authors found a long time tail in the velocity autocorrelation functions.⁽³⁾ The correlation functions are related to the viscosity. The results have indicated the necessity of sufficiently long time calculations of the motion of the atoms with the correlation of neighboring atoms in order to obtain transport coefficients in the statistical mechanics such as the diffusion coefficients or viscosity coefficients for realistic atoms or molecules.

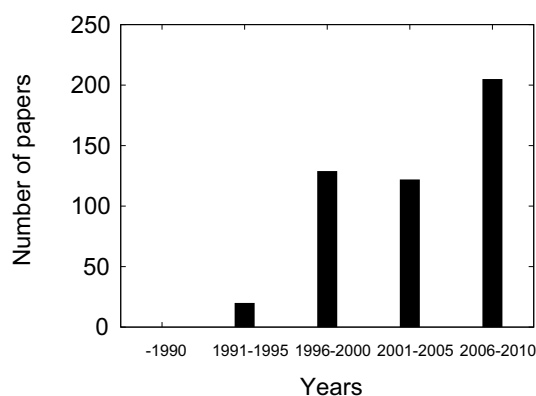


Fig. 1 Number of scientific articles concerning the molecular dynamics in tribology.

The simulations of the bulk viscous liquids became one of the main subjects in non equilibrium molecular dynamics simulations and were described in two books written by Allen & Tildesley⁽⁴⁾ and Evans & Morriss⁽⁵⁾ in 1987 and 1990, respectively.

The understanding of the molecular origin of the bulk viscosity of liquids is important but it is not enough. This is because tribology is surface science. Simulations of equilibrium structures of liquid molecules absorbed on the surface began to be studied around 1980.^(6,7) The fluidity of the absorbed molecules were studied. Analysis from the viewpoint of viscosity was discussed by Bitsanis et al. in 1987.⁽⁸⁾ They studied the dynamics of sphere-shaped Lennard-Jones particles confined between two parallel walls, and discussed the relation between the equilibrium structure and the viscosity including the effect of the boundary slip under a framework of the linear response theory.

A MD simulation of liquid molecules, which were constructed by 20 linearly connected sphere particles i.e., which had intramolecular degrees of freedom confined between two parallel walls and adopted shear by moving the walls was done by Thompson et al. in 1992.⁽⁹⁾ This work can be regarded as the completion of the foundation of the Tribo MD.

The friction coefficients can be considered as a type of transport coefficient.⁽¹⁰⁾ It can then be related to the energy dissipation due to the thermal vibration such as molecular motions under a weak external field. In other words, the molecular origin of frictions is related to the dissipation of the molecular motion energy responses to the external field produced by the sliding motion. The energy dissipation process can be described by classical molecular dynamics simulations.^(11,12) Adopting this idea to the analysis of MD simulations, the friction force changes by the specific molecular vibration mode within a huge relaxation mode of the molecular motion. In this paper, we review studies of non-equilibrium MD simulations of a traction fluid in a confined geometry, and analyze the energy dissipation processes due to this concept. Friction behavior of confined molecular layers differs when the molecules are governed by the main chain motion in the chain molecules, or the ring flap motion is incorporated in the ring molecules. In these simulations, the heat generated during the friction process is extracted by a heat bath, which is used to maintain the system at a fixed temperature.

If we cannot neglect the chemical reactions, the

friction dynamics can be analyzed by the non-classical or modified MD simulation. For example, the dynamics of an organic or inorganic film, which is chemically absorbed on the surface, the energy dissipates by the formation and disappearance of a chemical bond due to the friction. In order to investigate the mechanism of low friction of a DLC (diamond-like carbon coating) surface, the REBO (Reacting Empirical Bond Order) method, which is extended classical MD including bond exchanges due to a chemical reaction,⁽¹³⁾ or a tight-binding quantum MD method⁽¹⁴⁾ is used. If there are no chemical reactions, and no molecular internal degree of freedom, then the energy dissipation is due to lattice vibration in the solid.⁽¹⁵⁻¹⁷⁾

If we need to consider not only the atomistic motion, but also a structure change of some large molecules or flakes consisting of a large number of atoms, a coarse-grain molecular simulation is proper for the analysis. Recently, the ultra low mechanisms of solid layered graphites have been solved by coarse-grained molecular simulation, which is normally used to model soft materials such as polymers or liquid crystals.⁽¹⁸⁾ Each graphene sheet consisting of some hundreds to ten thousand atoms are modeled as a single coarse-grain sheet. The friction of layered materials is understood in the framework of the thermal escape motion of a transferred pile of graphene sheets. Energy dissipation is related to the dynamics of the structural changes of the coarse-grain sheets.

Although the extra simulational methods are presented to treat quantum mechanics or coarse-grain dynamics, the classical all-atom MD are effective method to analyze the tribological process. The analysis of traction fluids is one of the examples.

2. Traction Fluids and Elastohydrodynamic Lubrication

For fluids used in a traction drive type continuously variable transmission (CVT), its traction properties largely depend on the structure of the fluid molecules.^(19,20) In order to minimize and to achieve a higher CVT capacity, improved fuel economy and protect the environment, the molecular design on a molecular level of high traction coefficients is effective for the developments.

The lubrication condition of a working traction fluid is under elastohydrodynamic lubrication (EHL).^(21,22) On the other hand, the molecular mechanism of the

transmission of force in a highly-loaded fluid layer is not clearly known. Hence, the non-equilibrium MD simulations of a traction fluid in a confined geometry were investigated.⁽²³⁻²⁵⁾ The methods and some results are shown in the following sections. First, the fluid layer is confined between two solid plates under high pressure. The traction simulations are performed by applying a relative sliding motion to the solid layer. The mechanism of the traction due to the structure of the fluid molecules is finally analyzed.

Because of the large difference in the oil film thickness and shear viscosity, the simulations do not directly model the experiments.⁽²³⁻²⁷⁾ In most experiments, the film thicknesses are over $0.1 \mu\text{m}$ and the shear rates are below 10^6 s^{-1} . The film thickness regime in the simulations is far too thinner and the shear rate regime is far too higher than that in the experiments. Although recent hybrid simulations of the MD and computational fluid dynamics show the possibility of simulation under realistic shear rates and film thicknesses,⁽²⁸⁾ a simple method described in the next section is useful for survey.

The traction force of a fluid, which has the same definition as friction force, has its origin in the translational momentum transfer across the fluid layer. The traction force is generated by the momentum transfer between molecules from the viewpoint of the MD scale. At first, the external force, which is applied to the solid layer by a constant sliding movement velocity and normal constant pressure, transfers to the fluid molecules in the vicinity of the solid layer by an intermolecular interaction. The affected molecules deform their shape by an intramolecular interaction. The force transfers again to another molecule by an intermolecular interaction, and finally the force transfers to the other side of the solid layer as a traction force. The heat produced during this process dissipates to the bulk in each process. This process of momentum transfer should be treated as a statistical mechanical process, which is carefully extracted from the huge thermal noise. In order to solve this difficult problem, non-equilibrium MD simulations, which can treat a large number of fluid molecules up to a several hundred nm film thickness, are made using a supercomputer. The dynamics of several hydrocarbon fluids including industrial lubricant under shear and high pressure are then simulated. These test fluids have their own characteristic structures, and their traction coefficients were measured experimentally and compared to one another. The relation between the

obtained traction coefficients μ and molecular structure were then analyzed by focusing on the inter- and intramolecular interactions. The molecular mechanism of the traction phenomena in a fluid layer was then presented.

3. Molecular Dynamics Simulation

Figure 2 shows a schematic view of the Tribo MD. The all-atom modeled fluid molecules are dynamically treated using the AMBER force field.⁽²⁹⁾ The force field is described as a set of functions of two to four body interactions within each organic molecule of which the parameters are determined from ab initio molecular orbital calculations. On the x and y axes, the periodic boundary condition is adapted to the simulation cell, where x is the sliding direction and y is the direction of the fluid thickness.

The temperatures are controlled at 350 K using the Nosé-Höover formalism,⁽³⁰⁾ in which all the molecules are connected to a heat bath. While this model of a heat bath has been shown to affect the rheology of confined fluids at shear rates above $\dot{\gamma} = 0.2$ (in reduced Lennard-Jones units), the low shear rates here, a maximum of $\dot{\gamma}(\varepsilon / mR^2)^{1/2} \approx 0.004$, suggest that such artifacts should be negligible.^(31,32)

Each simulation step corresponds to 0.5 fs and the time integral due to the motion of the atoms is calculated by the rRESPA (Reversible Reference System Propagator Algorithm) method based on the velocity Verlet method for a time integral.⁽³³⁾

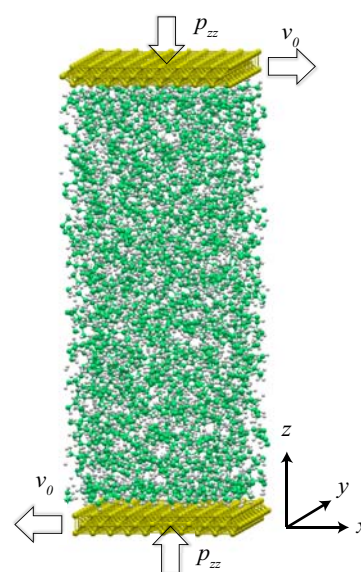


Fig. 2 Schematic view of Tribo Molecular Dynamics simulation.

The solid plate is modeled as an atom layer with a lattice of $100 \times 100 \times 3$ in the x, y, z directions and the lattice parameter is 2.87 due to the structure of an alpha-ferrous crystal. The fluid-solid interface faces the (100) surface, and the vibrations of each atom are suppressed.

The solid-fluid interaction is defined as a no-slipping condition by a sufficiently large interaction. This is because, under the EHL condition for a realistic submicron oil film thickness, the fluid-fluid interaction will be the origin of the traction appearance. The Lennard-Jones well depth parameter is then set to 12.14 kcal/mol. Under this condition, no slipping is observed.

Constant shear states under constant pressure and constant velocity are obtained in the following manner. First, a set of fluid molecules without a solid layer is arranged in a lattice configuration. The molecules are then relaxed by the MD simulation under the periodic boundary condition in the (x, y, z) direction at the constant temperature of 350 K until a thermal equilibrium is obtained. Next, the sets of thermal equilibrium fluids are arranged in the z direction between two solid layers. Fluid molecules are compressed by the MD simulation under the periodic boundary condition for the x, y direction by adopting the constant pressure of 1 GPa on the plates. The shear in the x direction is then applied by a relative sliding motion on the solid layers by the constant velocity. A judgment of the constant shear state is made by tracing the traction coefficients μ defined by

$$\mu = \sum F_{fluid}(x) / F_{ext}, \dots \dots \dots (1)$$

where $F_{fluid}(x)$ is the x component of the pressure on the plate from the plate-fluid interaction.

The traction coefficients μ increases first after the sliding starts, and then saturates to some fixed value and oscillates around this value at 50 ps from the beginning of the sliding, which corresponds to a constant shear state. The time average of μ is calculated from the average of μ within 5 ns of the constant shear state.

4. Molecular Structure and Traction Mechanism

4.1 Dependence of Traction Coefficient on Film Thickness and Shear Rate

The effects of the film thickness and shear rates on

the traction coefficient μ are first studied. To determine the condition that can qualitatively simulate the experiments, the dependence of μ on the film thickness was calculated. **Figure 3** shows the time average of the traction coefficient μ of n-hexane in the steady state in the film thickness range $z_0 = 1.0$ to 10.0 nm and in the shear rate range of $\dot{\gamma} = 1.0 \times 10^7$ to $1.0 \times 10^9 \text{ s}^{-1}$. Although the calculated traction coefficients show higher value than the experimental ones over the entire simulation range, μ decreased for both with the decreasing shear rates and increasing film thickness. This tendency provides a qualitative agreement with the experiments. In an ultrathin film less than 2.5 nm, a large stick-slip-like motion caused by slip between the molecular layers is observed, which suggests that a film thickness of at least 5.0 nm is needed.

4.2 The Effect of External Pressure and Phase Transition

The effect of the external pressure p_{zz} is studied by the large time scale simulations of 50 ns for each p_{zz} . In **Fig. 4.**, the dependence of the traction coefficient μ on the external pressure is plotted. The number of n-hexane molecules is fixed to 576 that corresponds to the film thickness of 10 nm at 1.0 GPa. The limiting shear stress transition of the traction coefficients is observed around 0.5 GPa to 1.0 GPa that corresponds to the phase transition from the viscoelastic region to the plastic-elastic region which was experimentally determined by Evans et al.⁽²²⁾

Molecular mechanisms of the phase transition are then analyzed by the radial distribution functions and the velocity profiles.⁽¹⁾ From the analysis, the transition is not only related to the arrangement of the molecules. The plasticity is also related to the suppression of the fluctuations in the molecular motion.

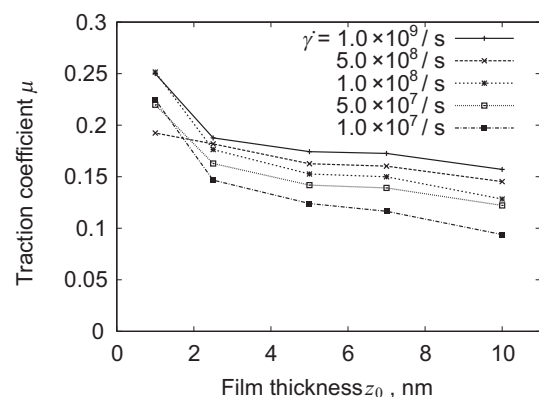


Fig. 3 Film thickness and shear rate dependence on μ .

4.3 Comparison of Experiments for Hydrocarbon Fluids

The MD simulations of 10 hydrocarbon fluids, which are composed of 6 to 18 carbon atoms, were examined as test fluids, their traction coefficients μ also measured by the disk on ball experiments and were compared to one another. The fluid molecules are A: *n*-Hexane, B: *n*-Hexadecane (chain molecule), C: Benzene (single ring aromatic molecule), D: Cyclohexane (single ring alicyclic molecule), E: tert-Butylcyclohexane, F: Methylcyclohexane, G: 1,4-Dimethylcyclohexane (single ring alicyclic molecule with side chain), H: Dicyclohexyl (dumbbell-like molecule made by two bound alicyclic molecules), I: Dicyclohexylmethyl (dumbbell-like molecule), J: Santotrac 50 (dumbbell like molecule, industrial traction lubricant).

In each simulation, the film thickness was fixed at 6.7 nm by fitting the number of fluid molecules. The sliding velocity was fixed to 1.0 m/s. **Figure 5** shows a comparison between the MD simulation and experiments. The simulated values of μ are always larger than the experimental values. This is because the film thickness on the simulation is too small compared to the experimental condition of a submicron thickness. Even if the absolute values are different, the order of μ according to the molecular structure is reproduced by the simulation.

The result supports the selection of the force field parameter, a sufficiently low shear rate, which can be achieved by the all atom MD simulations, a sufficiently large fluid thickness, which contains the bulk fluid layer region in the center of the film, an a

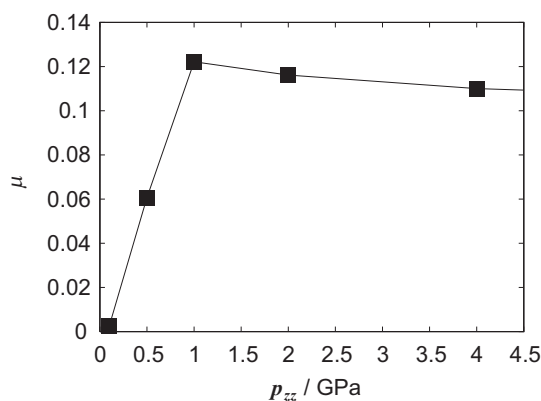


Fig. 4 External pressure dependence on film thickness and traction coefficients. *n*-hexane: 576 molecules, Sliding velocity: 1 m/s.

plate-fluid interaction in which the macroscopic interfacial slip is suppressed, which are correct and the simulation qualitatively reproduces the traction phenomena.

In both the MD simulation and experiment, the order of the traction coefficient depends not on the molecular weight, but the structure of the molecules, and seems to show the following tendencies.

1. Single ring alicyclic molecules show a large traction coefficient μ compared to the chain or aromatic molecules.
2. μ decreases with the substitution of a side chain.
3. If the side chain is an alicyclic residue itself (dumbbell-like molecule), μ does not decrease, but becomes larger than that for the mono-alicyclic molecule.

4.4 Structure of Oil Film

In order to investigate the order of the structure of the molecular layer, the molecular density profiles were plotted in **Fig. 6**. The molecular density is calculated from the density of the center of the mass in each molecule. The horizontal axis corresponds to the average film thickness, and the vertical axis corresponds to the average molecular density.

In the single alicyclic molecule D, the periodically layered structure is clearly constructed. That is, from the viewpoint of the structure of the fluid film, in molecule D, the molecules are well layered. On the other hand, the layered structure is not clear in chain molecules A and B, and the dumbbell-like molecules H, I and J. Therefore, each molecule is bridging the layers of molecules and the distribution is disordered.

We now discuss the relation between the order of the molecular layer and the mechanism of the momentum

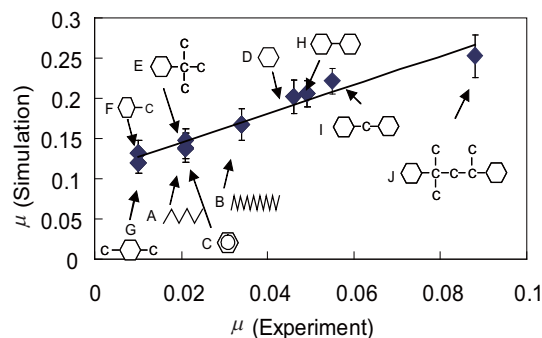


Fig. 5 Comparison of experiments (Film thickness $z_0 = 6.7$ nm, shear rate $\dot{\gamma} = 1.5 \times 10^8$ / s).

transfer in the fluid layer from the viewpoint of the MD scheme. In order to transmit the momentum from one atom to another, using a bonded interaction like a covalent bond has an advantage over using the nonbonded interaction like the van der Waals (Lennard-Jones) force. Therefore, if the molecular layers are disordered and each fluid molecule distributes across the layer, molecules would generate a high traction force in the entire system. Based on this hypothesis, the tendency of μ of $B > A$ in the chain-like molecules, and of $E, H, I, J > F, G$ in the alicyclic molecules, are able to be understood. The tendency that μ of molecule D is larger than that of A and E, however, cannot be explained from this point of view.

To analyze the condition of each molecule in the fluid layer, the orientation factor

$$\Phi = \left(3 \langle \cos^2 \theta \rangle - 1 \right) / 2, \dots \dots \dots (2)$$

is employed for the aromatic and alicyclic molecules. Here, θ is the angle between the normal to the plane of

the hexagonal ring of benzene and alicyclic products, and the z axis (direction of the film thickness), and is the average of all molecules. $\Phi = 1$: is completely oriented and $\Phi = 0$: is completely random.

The average orientation factor of each fluid molecule is shown in **Fig. 7**. When compared to molecule D, the orientation factor of molecule C is smaller. This is because in molecule D, the arrangement of the hexagonal rings face each other is stable, whereas, in molecule C, the T-shape conformation becomes much more stable than when facing each other.^(34,35)

Comparing the alicyclic molecules, the orientation factor decreases with the substitution of a side chain. The very low orientation factor values in molecules H, I and J reflect that in this molecule, the order of the molecular layer is low and the hexagonal rings are distributed across the layers, thus the hexagonal rings are hard to orient in the direction of the film thickness.

4.5 Intramolecular Interaction

The translational momentum transferred to the fluid molecule produces an internal distortion on the molecule by an intramolecular interaction. **Figure 8** shows the intramolecular interaction energy of the bond, bond angle, torsion (dihedral) angle of the 10 fluid molecules. Each intramolecular interaction

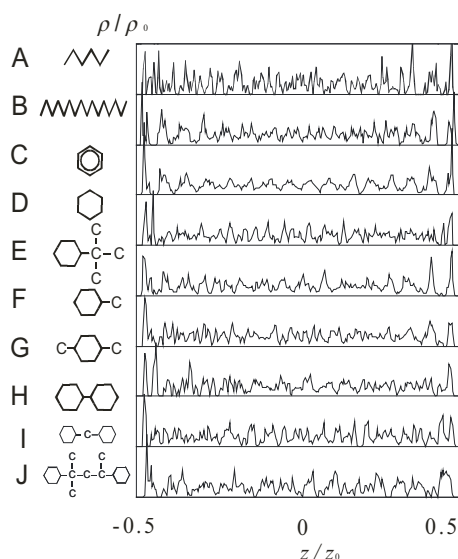


Fig. 6 Molecular density profiles.

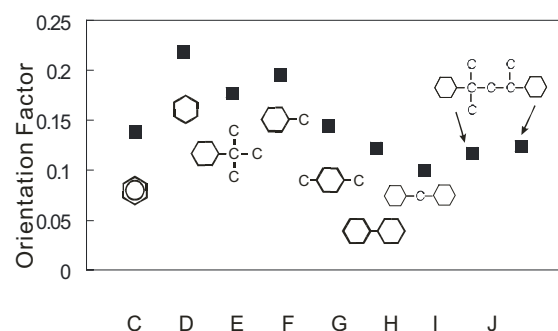


Fig. 7 Orientation factor of hexagonal rings.

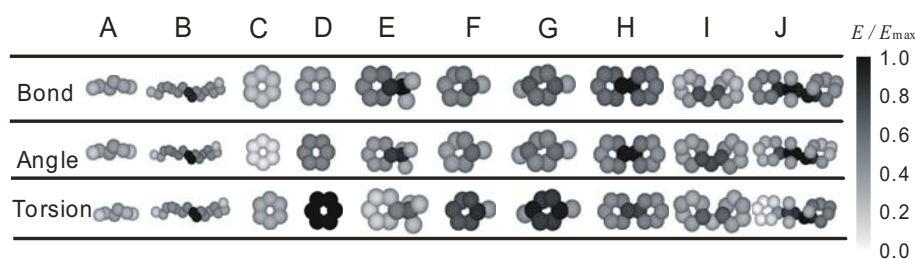


Fig. 8 Intramolecular energy on carbon atoms.

energy is normalized by dividing the energy by the maximum energy E_{\max} for all molecules of the bond, bond angle and torsion angle, respectively. E_{\max} for the bond and bond angle interaction is found in molecule J, and E_{\max} for the torsion interaction is found in molecule D. In chain molecule A, all the interaction energies of the bond, bond angle and torsion angle, have their peaks in the center of the molecule. The interaction energy in the aromatic molecule C is smaller than that of the alicyclic molecules which means that the distortion is low. In the alicyclic molecules, a large distortion is observed in the joint part of the substituted group. For any intramolecular interaction energy, the value of molecules A is quite low as is the distortion.

Comparing molecule D and the dumbbell-like molecules H, I and J, in molecules H, I and J, all the interaction energies are high in the joint part of the two alicyclic rings, so the distortion on the joint is the principal intramolecular interaction. On the other hand, the torsion angle energy is low in molecule D. This result suggests that the role of the hexagonal ring in the traction effect is different between molecule D and the dumbbell-like molecules H, I and J.

The hexagonal rings in the alicyclic molecules have a stable chair conformation, the boat conformation is unstable, and the chair conformation has axial and equatorial conformations which undergo rapidly changes of the so-called ring-flip.⁽³⁶⁾

For the stable chair conformation, the distance of a pair of carbon atoms on the opposite side is always greater than 2.7. We then defined the unstabilities of the alicyclic group as the ratio of the number of unstable rings divided by the number of whole rings, and plotted it in Fig. 9. Substitution on an alicyclic ring causes suppression of the mobility of the ring. The order of the instability corresponds to the order of the dihedral angle energy shown in Fig. 8.

Therefore, the mechanism for the high traction shown in molecule D, in contrast to the substituted molecules E, F and G, is due to the ring-flip motion of

the hexagonal rings facing together within the highly ordered and oriented molecular layer.

4.6 Intermolecular Interaction

According to the fluctuation dissipation theorem,⁽¹⁰⁾ shear viscosity is related to the correlation function of the momentum of the molecules generated in the absence of a shear field.⁽³⁷⁾ The mechanism of momentum transfer in the molecular layer is able to be analyzed by correlation functions. At every 25 ps, we numerically sorted the carbon atoms in increasing order of the distance from a carbon atom i , then correlation of the atom and the i th atom in the sorted list is calculated using the following equation

$$\langle p_x p_x(n) \rangle = \left\langle \sum_i p_{ix}(t) p_{ix}(t) \right\rangle_t / N, \dots \dots \dots (3)$$

where, $p_{ix}(t)$, and $p_{nx}(t)$ are the components of the momentum of atom i , n in time t , N is the total number of carbon atoms in the simulation cell, and $\langle \rangle$ is the time average. The partial correlation coefficient $C(k)$ is defined as the integral of the pair correlation functions $p_x p_x(n)$ with respect to n and subdivided the integral into the topologically different carbon atoms k on each fluid molecule, as shown in Fig. 10. All the

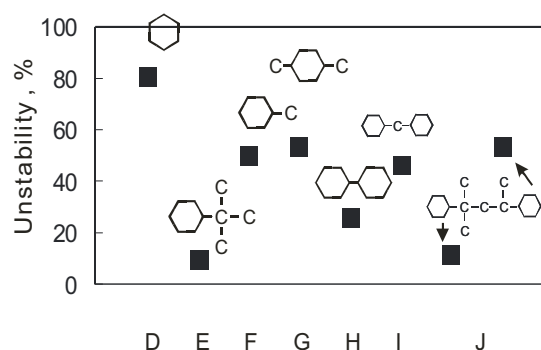


Fig. 9 Unstabilities of an alicyclic group.

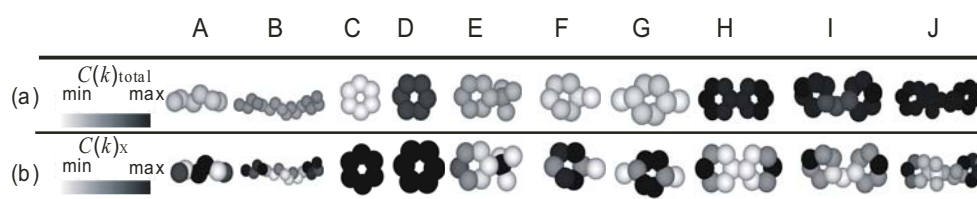


Fig. 10 Pair correlation coefficients.

values of $C(k)$ in Fig. 10 (a) are normalized by the maximum value of the 10 hydrocarbon fluids, $C(k)_{total}$.

Comparing chain molecule A and the dumbbell molecules H, I and J, a small deviation in molecule A is found whereas a large value in both ends of the molecule is found in molecules H, I and J which means the molecular motion works together with the other molecule at both ends of the molecules.

Comparing the momentum transfer among the alicyclic molecules, in contrast of the case that in molecules H, I and J, for the momentum transfer on both ends, the maximum values are observed in the center of molecules and the momentum transfer is low at both ends in the case of F and G. The bicephalous properties (the center part of the momentum transfer is divided into two parts in the molecule) are found in molecule E, and this tendency becomes clear in molecules H, I and J. The pseudo bicephalous properties shown in molecule B should be attributed to the decreasing number of surrounding molecules in the middle of the long chain.

4.7 Molecular Mechanism of Traction

Based on the above results and analysis, we propose the origin of traction in the fluid layer as follows:

1. If the order of the molecular layer is low (disordered), fluid molecules distribute across the layers, and the fluid shows a high traction. Therefore, the tendency of μ in chain molecules $B > A$, alicyclic molecules $E, H, I, J > F, G$ can be explained from this point of view.
2. The reason that within the alicyclic molecules, molecule D shows a high traction coefficient μ than the others, is due to the ring-flip motion of the hexagonal rings facing together within the highly ordered and oriented molecular layer.
3. The high traction coefficients of the dumbbell like molecules H, I and J compared to E, F and G occur because the fluid molecules in which the hexagonal rings distribute across the disordered molecular layer transmit the momentum at both ends of the molecule in the bulk. The reason why molecule E, which is close to the bicephalous property of molecule H, shows a higher traction coefficient, and molecule B, which does not have the bulk part of that in F and G, shows a lower traction coefficient than H can also be understood.
4. The reason why the traction coefficient of the alicyclic molecule D has a higher value than the

aromatic molecule C is due to its origin in the presence of the ring-flip motion, the same as 2.

5. Conclusions

The simulations of the all-atom molecular dynamics were performed to analyze the molecular mechanism of the EHL oil film. From the analysis of the film thickness, the results suggest that the MD simulations provide reliable results for the films thicker than 5 nm to explain the behavior of groups of molecules in actual phenomena. The phase condition of the oil film under 1 GPa is in the elastic-plastic region which was confirmed from the existence of the limiting shear stress. During the course of the MD simulation of traction fluids, the order of the traction coefficients of 10 hydrocarbon fluid molecules using disk on ball experiments are reproduced. The mechanisms of the traction are analyzed from the viewpoint of the relation between the translational momentum transfer across the fluid layer and inter- and intramolecular interactions. In the dumbbell-like molecules, alicyclic rings, which distribute across the low ordered molecular layers, behave as a stiff bulky mass, and the momentum transfers to the end of the molecular axis. The origin of the traction generated in the fluid layers is clarified.

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Fig. 1

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Fig. 3

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Fig. 4

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Figs. 5-10

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Sections 3 and 4.3-4.7

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