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Molecular Dynamics Simulation for Analysis of the Behavior of Organophosphate Aggregates in Oil

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Organophosphates are representative compounds of extreme pressure additives. Our previous study [1] have shown that they form aggregates and weakly attract on solid surface under the ambient pressure. In order to further understand their behavior in oil, we compare the diffusivity of organophosphates and base oil. The results show that the diffusivity of the organophosphates on short time scales is affected by the number of alkyl chains, but on long time scales, the differences in the number of those does not affect the diffusivity when the hydrodynamic radius of organophosphate aggregates is almost the same.

Keywords (from 3 to 5 max): nanotribology, lubricants, extreme pressure additive, molecular dynamics

1. Introduction

Oiliness improver and extreme pressure additive are representative of additives for machine oil. Although, the fatty acids and the organophosphates have similar physicochemical structures with alkyl chains attached to polar groups, the tribological usage is very different, i.e. the latter acts in severe condition such as high temperature and heavy load. In this study, in order to clarify their molecular features, we analyze the mechanics of organophosphates in base oil by molecular dynamics simulations, and compare it with our previous study [2] of the effect of fatty acids in base oil.

2. Methods

In this study, MD calculations are performed for a material system in which the base oil is 3,5-diethyldodecane (DED) and the extreme pressure additives are monooleylphosphate (MOP) or dioleylphosphate (DOP). Figure1 shows the structures of these molecules. The simulation cell consists of 96 molecules of DED and 4 molecules of MOP or DOP, under the periodic boundary conditions in the x, y, and z directions. The Dreiding force field is applied to the intermolecular and intramolecular interactions, and the charges of each atom are obtained by the molecular orbital calculation using MOPAC6. MD calculations are performed under NVT conditions, and the temperature is controlled to 350 K using the Nosé-Hoover method. The long-range Coulomb force is evaluated using the multi summation method, and the cutoff distance of the short-range interaction is 15 Å. The time steps are set to 2 fs, and the equation of motion is integrated using the velocity Verlet method. These MD calculations are performed using LAMMPS (3Mar20 version.).

3. Results and Discussions

Figure 2 shows the mean square displacements (MSD) of organophosphates and base oil in systems with additives of MOP or DOP and without additives. On short time scales, MOP is more diffuse than DOP, which can be understood to be due to the differences in the number of alkyl chains. In contrast, there is no significant difference

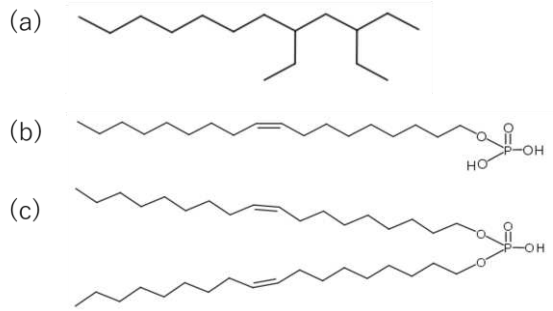

Figure 1: Molecular structures of (a) DED, (b) MOP, and (c) DOP.

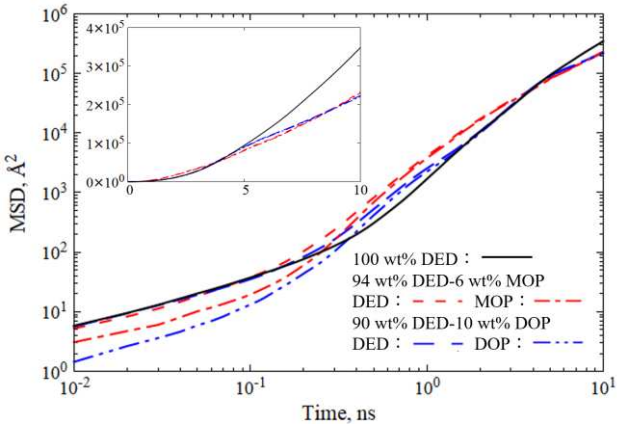

Figure 2: Mean square displacements of organophosphate molecules and base oil molecules obtained by the MD calculation.

in the diffusivity of MOP and DOP on long time scales. It is inferred that this is because the hydrodynamic radius of the organophosphates as they form aggregates is almost the same.

4. References

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