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Multi-physics and chemical understanding of boundary lubrication using molecular based simulations

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In this paper we summarize our recent finding concerning about boundary lubrication using multi-physics approach with molecular dynamics simulations. The early physical adsorption process is studied for friction modifier, extreme pressure agents are studied and the physical-chemical difference between the behavior in the oil of two additives are clearly characterized. Using reaction force field, mechanism of selective adsorption of anti-corrosion additives on the newly formed metal surface is found. Formation process of the transfer layer of friction of diamond-like carbon or metal with zirconia is detected. These findings contribute to coarse-grained or meso-scale simulations.

Keywords: multi-physics simulation, boundary lubrication, adsorption, surface interaction

1. Introduction

Friction, wear and lubrication is in principle multi-scale and multi-phyisics phenomena. This is because these tribological properties are not determined by a property of a single material. In this paper we report our recent finding on boundary lubrication in both physical and chemical molecular simulation and consider the way to attack more integrated phenomena by multi-scale simulations.

2. Physical adsorption and long-range interaction

The effect of structure of base oil molecules on oiliness agents (friction modifier) are mainly studied under the concept of "chain matching". In order to understand the phenomena by molecular dynamics simulation, we found that, in the early physical adsorption process, the base oil molecule prohibit the adsorption by layering on the solid surface [1]. The result suggest that the structure of base oil is important to determine the time constant and physical properties of surface boundary layer.
In the similar simulation for organophosphates as extreme pressure additives, we found that the EP molecules aggregate in the base oil and make reverse micelle, which do not adsorb on the solid surface in room temperature without external perturbation [2]. This means that the long-range Coulomb interaction between functional groups are very important in low permittivity solution such as lubrication oil environment.

3. Chemical adsorption and transfer layer formation

Chemistry is also important to understand the boundary lubrication. In order to show the mechanism of selective adsorption of newly formed copper surface by anti-corrosion additives, the simulation of adsorption process on hybrid surface (solid slab of both oxidized and not-oxidized copper) is studied using reacting force field [3]. Then we found that in the beginning, the additive adsorb in both surface, but after then a molecules adsorbed on the newly formed metal obtain electrons from the surface and due to the increase of polarizability, the molecules interact strongly with the other molecules and at final, the molecules cover the newly formed surface. This mean the change of polarizability must take into account to understand the selective adsorption phenomena. The importance of charge transfer is also found on the formation process of formation process of transfer layer made by ethanol on the zirconia surface [4].

4. Multi-scale simulations for boundary lubrication

In order to reflect the knowledge to the multi-scale simulation, we are constructing two types of simulator in submicron scale and in micron scale. For the submicron scale, multi-physics simulator is constructed [5]. In this simulator, the motion of coarse-grained molecules is treated by Langevin equation and the flow of base oil is treated by Lattice Boltzmann method solving Navier Stokes equation. In the coarse-grained molecules, the functional groups of the molecules are included from bottom up method [6]. For the micron scale, multi-physics simulator based on smoothed particle hydrodynamics is presented [7]. In this simulator we can calculate friction, partial heat generation and transfer, surface interaction calculated from molecular model, third body effect, and anisotropic particle model in order to calculate large system in aspect ratio such as tribological system.

5. References

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