# 反応力場と古典力場による極圧添加剤の分子動力学解析

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Molecular Dynamics Analysis of Extreme Pressure Additives using Reactive and Classical Force Field ([1]*Graduate School of Information Science, University of Hyogo*, [2]*Idemitsu Kosan Ltd.*) ○Hitoshi Washizu[1], Kyosuke Kawakita[1], Yuki Iike[1], Mutsuki Homma[1], Riku Araki[1], Yoshiki Ishii[1], Hiroaki Koshima[2]

The extreme pressure additives in lubrication oil make surface film reacting on the metal surface under high temperature and high share and bring low friction and wear. The mechanism is not easy to understand since they include many process. Additive molecules make reverse micelle in normal condition. Then the molecules adsorb on metal surface under lubricating condition. We used molecular dynamics simulation to understand the stability of reverse micelle in room temperature. Then used reactive force field to analyze surface reaction on metal surfaces and results revealed the mechanism.
*Keywords : Molecular Dynamics, Extreme Pressure Agent, Friction, Wear, Reverse Micelle*

潤滑油の添加剤[1,2]の中でも，極圧添加剤についての理解は大変難しい．これは，高温，高せん断の曲圧状態において金属表面において化学反応により皮膜を形成し，低摩擦および低摩耗を実現するためである．我々は，古典力場を用いて常温において極圧剤が作用しない理由，すなわち逆ミセル形成による安定化について検討した．次に，反応力場を用いて金属および金属酸化物表面における反応を解析し，分子形状の違いによる物理・化学吸着挙動の発現機構について明らかにした．

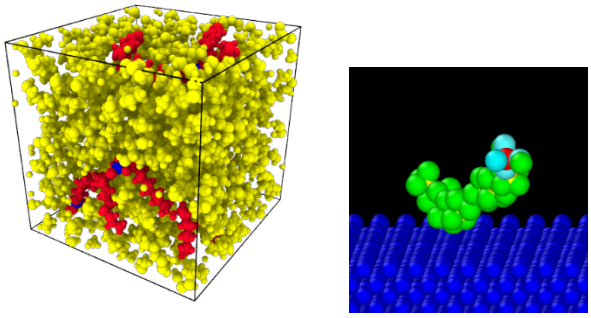

Fig. 1 Molecular dynamics simulation of mono-Oleyl phosphate. Classical molecular dynamics of reverse-micelle formation (left) and reactive molecular dynamics of surface adsorption (right).

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2) K. Nishikawa, H. Akiyama, K. Yagishita, H. Washizu, *Jurnal Tribologi,* **2019**, 21, 63.