Development of Multi-level Tribological Simulator based on Ultra-accelerated Quantum Chemical Molecular Dynamics

Akira Miyamoto

(Tohoku University, New Industry Creation Hatchery Center, Professor)

【Outline of survey】

It is urgent to develop alternative lubricant that does not contain sulfur and phosphorus from the point of view of environmental friendly and achievement of reliable mechanics. Therefore, it is strongly demanded to establish the novel methodology to investigate dynamics behavior of lubricant as well as involved chemical reaction in nano space under friction. This needs deeply understand of fundamental of conventional additive in a lubricant and anti-wear phenomena. We have successfully developed tribochemical simulator, “Hybrid-Colors”, which enables to simulate mechanical friction with consideration of chemical reaction. On the other hand, we have recently developed ultra-accelerated quantum chemical molecular dynamics that is faster by 10 million in computational speed than conventional first-principles molecular dynamics. In this study, we challenge to develop “Multi-level Tribological Simulator” based on the ultra-accelerated quantum chemical molecular dynamics and recently developed simulators related to the tribology, which makes possible to investigate the phenomena observed in tribology field from electronic-level to macroscopic-level.

【Expected results】

In this study, “Multi-level Tribological Simulator” is developed based on both an ultra-accelerated quantum chemical molecular dynamics and recently our developed simulators. This simulator models chemical reaction under friction from electronic-level to macroscopic-level. Moreover, several utilization tools for this simulator such as potential parameter fitting simulator based on precise quantum mechanics are also developed. This developed simulator is verified by applying to practical problem of mechanochemical reaction, e.g. lubricant additive for automobile, and comparing with the experimental observation.

【References by the principal investigator】

・Michihisa Koyama, Jun Hayakawa, Tasuku Onodera, Kosuke Ito, Hideyuki Tsuboi, Akira Endou, Momoji Kubo, Carlos A. Del Carpio, and Akira Miyamoto, “Tribochemical Reaction Dynamics of Phosphoric Ester Lubricant Additive by Using a Hybrid Tight-Binding Quantum Chemical Molecular Dynamics Method”, J. Phys. Chem. B, 110 (2006) 17507-17511.

・Yusuke Morita, Tasuku Onodera, Ai Suzuki, Riadh Sahnoun, Michihisa Koyama, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou,Hiromitsu Takaba, Momoji Kubo, Carlos A. Del Carpio, Takatoshi Shin-yoshi, Noriaki Nishino, Atsushi Suzuki, Akira Miyamoto, “Development of a New Molecular Dynamics Method for Tribochemical Reaction and its application to formation dynamics of MoS_2 tribofilm”, Appl. Surf. Sci., in press.

【Term of project】 FY2008－2012	【Budget allocation】 153,600,000 yen (direct cost)

【Homepage address】 http://www.aki.che.tohoku.ac.jp/index-j.html