Development of Tribochemical Reaction Simulator Based on Hybrid Quantum Chemical Molecular Dynamics Method

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

【 Outline of survey 】

Recently, much attention has been given to the friction and lubrication processes in the nano-level confined system, namely the nano-tribology processes, because of the severe requests to the environments, energy conservation, down-sizing, and so on. Hence, recently we have succeeded in the development of tribology simulator "TRIBOSIM", which can clarify the tribology process at atomic level, based on classical molecular dynamics method. It realized to predict various physical properties of lubricants and to reveal the friction and lubrication mechanism. On the other hand, more recently electronic clarification of the tribology processes including the chemical reactions, namely the tribo-chemical reactions, is strongly demanded. However, there is no theoretical simulator, which can clarify the tribo-chemical reactions in the world. Hence, in the present project, we plan to integrate our original tribology simulator "TRIBOSIM" based on classical molecular dynamics method and our original accelerated quantum chemical molecular dynamics simulator "Colors" based on SCF-Tight-Binding theory and to develop a tribo-chemical reaction simulator "Tribo-Colors", which can clarify the chemical reaction dynamics under the tribology processes. Moreover, we will apply our new program to the theoretical design of various tribology materials and processes.

【 Expected results 】

There is no theoretical simulator, which can clarify the tribo-chemical reactions, since both the chemical reactions and mechanical frictions should be simulated at the same time. In the present project, a tribo-chemical reaction simulator "Tribo-Colors" will be developed for the first time in the world. This new simulator enables us to realize the theoretical design of various tribology materials and processes on electronic level, in which the tribo-chemical reactions play important roles. Moreover, quantum chemical molecular dynamics approach, which has been developed in the chemistry field, will be applied to the mechanical engineering field for the first time. This new approach will innovate new research area in the mechanical engineering field.

【 References by the principal researcher 】

(1) H. Zhou, P. Selvam, K. Hirao, A. Suzuki, D. Kamei, S. Takami, M. Kubo, A. Imamura, and A. Miyamoto, Development and Application of a Novel Quantum-Chemical Molecular-Dynamics Method for Degradation Dynamics of Organic Lubricants under High Temperatures and Pressures, Tribology Lett., 15 (2003) 155-162.
(2) D. Kamei, H. Zhou, K. Suzuki, K. Konno, S. Takami, M. Kubo, and A. Miyamoto, Computational Chemistry Study on the Dynamics of Lubricant Molecules under Shear Conditions, Tribology Intern., 36 (2003) 297-303.

【 Term of project 】 F Y 2004 — 2008 | 【 Budget allocation 】 87,400,000 yen

【 Homepage address 】 http://www.aki.che.tohoku.ac.jp