

【Grant-in-Aid for Scientific Research(S)】
Science and Engineering (Engineering)



Title of Project : Development of Experiment- and Measurement- Integrated Multilevel Tribology Simulator Based on Accurate Modeling

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Research Area : Mechanical Engineering

Keyword : Tribology, Computational Chemistry

【Purpose and Background of the Research】

In addition to the multilevel tribology simulator developed so far, recently methods for instrumental analyses and measurement tests in the tribology field have been progressing dramatically. Against that background, the experiment-integrated multilevel tribo-simulator (Fig. 1) is developed by combining the multilevel simulation with tribology analyses, tribology measurements and tribo-components simulations. The powerful methodology supporting the tribological engineering in the future will be built from the synergy of experimental research handling real materials and conditions with theoretical research centering on quantum chemistry.

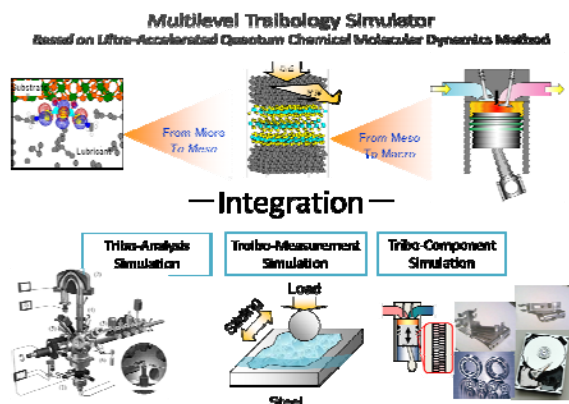


Figure 1 Simulation Scheme

【Research Methods】

In the present research, the following six subjects are conducted: (1) development of computational modeling technique of the real structure appearing in tribology experiments, (2) development of the theoretical prediction method of the tribological physical properties based on (1), (3) development of the tribo-measurement and the tribo-test prediction method built-up from an atomic level, (4) development of the prediction method of friction and wear behavior for the tribo-components and tribo-apparatus built-up from an atomic level, (5) development of the human interface for cooperation with experimental researchers, and (6) validation

and subject extraction of the developed simulator in cooperation with the experimental researchers.

【Expected Research Achievements and Scientific Significance】

The novel research method, “experiment- and measurement-integrated multilevel tribology simulator based on accurate modeling” in which the experimental techniques of tribo-analyses, tribo-measurements and tribo-components are integrated in, is to be established. By this research, if various measurement- and experiment-integrated multiscale tribology simulators are completed, it not only provides the powerful tool with which one can analyze and design the important tribological issues such as next-generation automobiles, medical equipments and so on, but also it will be highly-influential on the future mechanical engineering research. Because “tribology” is the research area linking academics and social needs, it is expected that the impact to other significant industries spreads.

【Publications Relevant to the Project】

- J. M. Martin, T. Onodera, M.-I. De Barros Bouchet, N. Hatakeyama, A. Miyamoto, “Anti-wear Chemistry of ZDDP and Calcium Borate Nano-additive. Coupling Experiments, Chemical Hardness Predictions, and MD Calculations,” *Tribol. Lett.*, 50, 95-104, (2013).
- Y. Morita, S. Jinno, M. Murakami, N. Hatakeyama, A. Miyamoto, “A Computational Chemistry Approach for Friction Reduction of Automotive Engines,” *Int. J. Engine Res.*, (2013), in press.

【Term of Project】 FY2013-2017

【Budget Allocation】 167,400 Thousand Yen

【Homepage Address and Other Contact Information】

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