Development of Multi-scale, Multi-physics Simulators for TribochemicalApplications

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1. Introduction

The design of tribological systems has provided a variety of technological challenges to experimental researchers. For computational or theoretical chemists tribological systems have given a variety of theoretical challenges to contribute more from theoretical or computational view-points.In collaboration with experimental experts we have developed manytribologicalsimulators[e.g.1-3]. The Ultra-Accelerated Quantum Chemical Molecular Dynamics(UA-QCMD) method is very useful for tribo-chemical simulations and multi-scale. multi-physics tribological simulations because the UA-QCMD method can perform quantum molecular dynamics calculations 10,000,000 times faster than a conventional first principles molecular dynamics method under similar conditions[e.g.4-6]. We have also demonstrated that the UA-QCMD has accuracy as high as that of first-principles or thermodynamics calculations. On the basis of such progress in microscopic, mesoscopic, and macroscopic simulators. we have attempted in the present study to develop multi-scale, multi-physics simulators for a variety of tribochemical applications..

2.Computational methods

Details of various simulators including UA-QCMD, mesoscopic simulators and tribochemical simulators, thermal conductivity simulator, electrical conductivity simulator are described in our previous papers [e.g.1-12].

3.Results and discussion

In our previous studies the UA-QCMD method with the first-principles parameterization is 10,000,000 times faster than the conventional first principles molecular dynamics method[4-6].We also demonstrated that the quantum chemical calculation in UA-QCMD, that is Colors, has high accuracy in comparison with DFT and thermodynamic data.In addition to the high accuracy in binding energy calculations, the UA-QCMD method can quantitatively reproduce the electron configurations of DFT calculations for various compounds. It should also be noted that the UA-QCMD is very effective for electronic calculations of rare earth compounds with f-orbitals, while the DFT method cannot reach divergence easily and thus cannot converge for these compounds.

On the basis of high speed and high accuracy the UA-QCMD methodhas revealedthe dynamic structure changes under tribological conditions. The validity of the dynamic calculations can be proved by simulating various spectroscopic results coupled with the comparison with experimental measurements. The precise determination of the geometry has determined nano-scale physical properties for mesoscopic and macroscopic tribologicalsimulations(Fig. 1). The results of such multi-scale, multi-physics simulation agree with various macroscopic measurements.

We plan to demonstrate that many important tribochemical phenomena can be simulated with the combination of various softwaresincorporated in the multi-scale, multi-physics simulators.

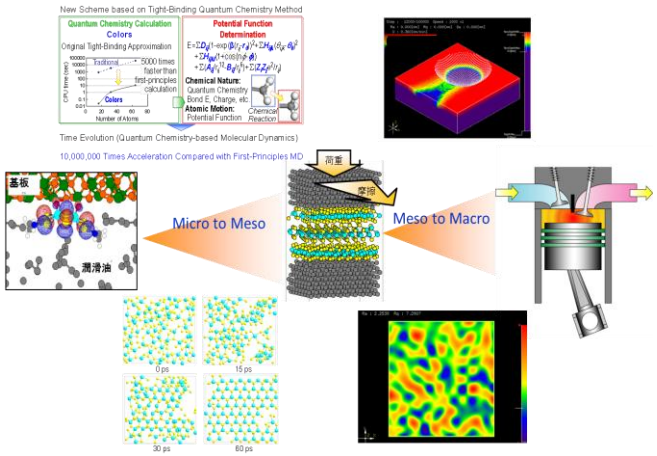

Fig.1 Multi-scale, multi-physics tribological simulators based on the UA-QCMD method

4. References

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