Multi-Physics and Multi-Chemistry Simulations on Friction and Wear Processes of Diamond-Like Carbon Films

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Super-low friction properties of materials are strongly desired for automotive engines and equipment in the sight of energy saving and efficiency. Recently, diamond-like carbon (DLC) films have gained much attention as super-low friction materials. Experimentally, it is pointed out that multi-physics and multi-chemistry processes are entangled in the friction processes of the DLC films and they lead to the difficulties in the clarification of the super-low friction mechanism of the DLC films. Moreover, in order to industrialize the DLC materials, the minimization of the wear in the DLC films during the friction processes are important. However, the wear processes are also multi-physics and multi-chemistry processes and then the elucidation of the wear processes of the DLC films are more difficult. Therefore, we have developed tight-binding quantum chemical molecular dynamics and reactive molecular dynamics simulators to clarify the multi-physics and multi-chemistry processes in the tribology processes and these simulators were already successfully applied to various multi-physics and multi-chemistry processes in tribology fields [1-3].

Fig. 1 shows the simulation model for the wear processes of the DLC films during the friction processes by our reactive molecular dynamics simulator. We observed the generation of the organic molecules such as methane, ethane, ethylene, etc. by the complicated tribochemical reactions. The product compositions are in good agreement with the experiments. Furthermore, we simulated the effects of the environments such as H_2 and H_2O conditions on the fricition and wear processes. We also elucidated that environmental conditions strongly affect the tribochemical reaction dynamics and wear products of the DLC films. In this conference, we will introduce our recent approaches to the multi-physics and multi-chemistry dynamics in the friction and wear processes of the DLC films.

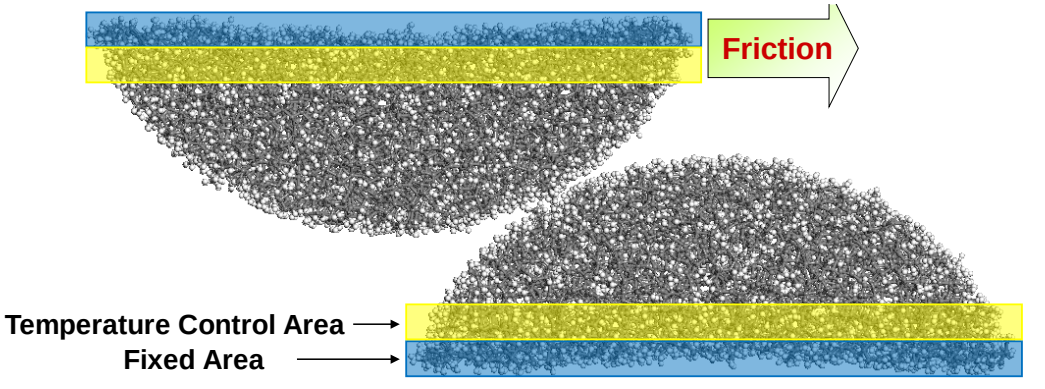

Figure 1: Simulation model for wear processes of DLC films during the friction processes

Reference:
[1] M. I. De Barros Bouchet, J. M. Martin, J. Avila, M. Kano, K. Yoshida, T. Tsuruda, S. Bai, Y. Higuchi, N. Ozawa, M. Kubo, and M. C. Asensio, **Sci. Rep.**, 7 (2017) 46394.
[2] K. Kawaguchi, H. Ito, T. Kuwahara, Y. Higuchi, N. Ozawa, and M. Kubo, **ACS Appl. Mater. Interfaces**, 8 (2016) 11830.
[3] T. Onodera, T. Nakakawaji, K. Adachi, K. Kurihara, and M. Kubo, **J. Phys. Chem. C**, 120 (2016) 10857.

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