Chemical Reaction of Alcohol due to Friction between Zirconia and Metal

Yosuke Hamano [1)] Hirotoshi Akiyama [1)], Yoshiki Ishii [1)], Hitoshi Washizu [1)]

[1] University of Hyogo
Corresponding author: h@washizu.org

The frictional fade-out (FFO) is the phenomenon of a significant decrease in the coefficient of friction between zirconia (ZrO_2) and diamond-like carbon (DLC) when they are exposed to a special environment [1]. The characteristics of ZrO_2, which is catalysis of hydrogenation of ethanol molecules in their environment, have a significant influence on the conditions for the phenomena of FFO to make a boundary tribofilm. In this study we report by a molecular dynamics simulation that, a similar phenomenon as FFO may be confirmed when conditions for FFO are met even if the counter material of ZrO_2 is other than DLC.

Keywords: Frictional Fade-Out, Zirconia, Polymerization Reaction

1. Introduction

Friction fade-out (FFO) is phenomenon that friction coefficient drops to 0.0001 when ZrO_2 slide against Hydrogen contain diamond like carbon (DLC) in a specific environment. The characteristics of the ZrO_2, which is catalysis of hydrogenation, have a significant influence on the conditions for the phenomena of FFO [2]. In this study, instead of DLC, Ni is employed as counter materials and the formation process of Tribofilm (polymer transfer layer), which is essential for FFO is studied by reactive molecular dynamics simulation.

2. Methods

Figure 1 shows the Snapshot of the MD cell after 500 ps slide. Since the zirconia used in the experiments is yttria-doped stabilized zirconia, YSZ is also used in this simulation. YSZ is placed in the upper part of the simulation cell and Ni solid slab is placed in the lower part. Ethanol and hydrogen radicals are placed between the sliding surfaces. In this study, it is assumed that ethanol is encapsulated from the atmosphere at the point where the hydrogen molecule dissociates first and becomes a radical, in order to make the simulation more efficient. The YSZ is sliding along the Z-axis at a speed of 100 m/s while applying 2.5 GPa of pressure in the Y-axis direction. Previous studies have confirmed that there is no correlation between the sliding speed and the frequency of polymerization [3]. In order to stabilize the model, the movement of the atoms is fixed in the direction of the film thickness by 3.0 Å at a distance from the sliding surface.

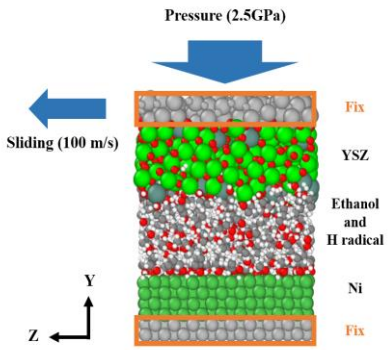

Figure 1: Snapshot of the MD cell after 500 ps slide.

3. Result and Discussion

Table 2 shows the chemical species produced after the sliding at 100 ps and 500 ps (Fig. 1). Comparing the results for DLC and Ni, polymerized hydrocarbon polymerized molecules are also observed in the case of Ni. In addition, the number of hydrocarbon molecules that polymerize over time is increasing. Furthermore, the results of chemical reactions of alcohols are studied. An oxygen atom in YSZ is bound to a carbon atom in the ethanol molecule. Both alcohol polymerization and adsorption to the YSZ occur via dehydrogenation. First, hydrogen-radical is adsorbed on ethanol molecule's oxygen atom. Second, water molecules are released from C_2H_5 due to the sliding. Finally, C_2H_5 are combined with the oxygen atom of the ethanol molecule or the oxygen atom of YSZ. These reactions are occurring at the YSZ surface and are thought to be influenced by the catalytic action of YSZ. This phenomenon may correspond to the initial process of polymerization of Tribofilm.

Table 2: Table of reaction products

	Time[ps]	C_2H_6O	H	$C_4H_{11}O$	C_4H_{10}
DLC	0	244	244	0	0
	100	200	11	1	1
Ni	0	244	244	0	0
	100	207	60	1	0
	500	207	98	2	2

※Only the polymerized hydrocarbon molecules are shown. There are chemical species that are omitted.

4. References

[1] M.Nosaka et al., "The Run-in Process for Stable Friction Fade-Out and Tribofilm Analyses by SEM and Nano-Indenter", Tribology Online Vol.12(5), 274-280(2017).

[2] Y.Tsutomu, "Application of ZrO2 as a catalyst and a catalyst support", Catalysis Today, Vol 20, Issue 2, 29 June 1994, Page 199-217

[3] R. Nakae, H. Washizu, "Molecular Dynamics Simulation of Polymerization in Solid Friction using Reactive Force Field", International Tribology Conference Sendai 2019, Sendai, Japan, 21-G-11 (2019).