EFFECT OF ENVIRONMENTAL GAS AND ITS HUMIDITY ON FRICTION OF CNx COATINGS SLIDING AGAINST Si3N4 BALL

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ABSTRACT

The friction test of CNx coatings sliding against Si3N4 balls showed the increasing of friction coefficient with humidity. To clarify the mechanism of the effect of humidity on friction property of CNx, we observed the transfer layer on Si3N4 balls after sliding tests in dry N2, air with humidity and N2 with humidity. The average physical adsorption structure of H2O on sp2-carbon containing nitrogen was estimated by using the orbital of density functional theory calculations. From the change of transfer layer and the physical adsorption structure of H2O, we discuss the effect of humidity on the friction property of CNx.

Keywords: CNx, friction, transfer layer, humidity.

INTRODUCTION

CNx coating sliding against Si3N4 ball had shown an ultra low friction coefficient less than 0.01 under dry N2 [1]. The transfer layer formed on Si3N4 ball during sliding tests under dry N2 had been reported [1]. On the other hand, CNx coating sliding against a Si3N4 ball under humidity had shown the increasing of friction coefficient [1]. It can be considereds that the humidity in environmental gas caused the decrease of transfer layer and the increase of friction coefficient during sliding against Si3N4 ball. But we did not observe the change of transfer layer under the environmental gas with humidity. To clarify the effect of the humidity on the increase of friction coefficient, we believe that the physical adsorption structure between water molecule and CNx are important. In the present study, we carried out the friction tests in N2 with humidity and in air with humidity. The transfer layers on Si3N4 balls after sliding tests were investigated, respectively. The physical adsorption structure of water molecule on sp2-carbon containing nitrogen were estimated using the orbital of density functional theory calculations. From the change of transfer layer and the adsorption structure of H2O, we discuss the effect of humidity for the increase of friction.

EXPERIMENTAL AND THEORETICAL CALCULATIONS

We used ion beam assisted deposition to deposit a CNx coating layer on a Si substrate [1] and amorphous carbon (a-C) coating layer, respectively. Deposition time was calibrated to control the thickness of 160nm. The other deposition conditions are described in Reference [1]. Next, the friction tests were carried out in a pin-on-disk tribometer. The sliding test conditions of the CNx coating and the a-C coating were shown in Fig. 1. To investigate the physical adsorption structure of water molecule between disk side and ball side, the structure of H2O on CNx was examined using the orbital of density functional theory calculations. The charge-neutral hexamer of prism type, 6H2O on sp2-carbon containing nitrogen, C46N2H24 (Fig. 2,
were prepared. The geometries of 6H$_2$O on C46N2H24 was fully optimized at the WB97XD/6-31G** level of theory. In this works, the calculation and the visualizing the model were performed with the program GAUSSIAN 09 suite [2] installed on a Fujitsu PRIMERGY CX400 computer at the Information Technology Center of Nagoya University.

RESULTS AND CONCLUSIONS

Friction properties of CNx and that of a-C are shown in Fig. 1. Friction property of CNx showed an ultra low friction coefficient less than 0.01 in dry N$_2$. The transfer layer formed on Si$_3$N$_4$ ball. On the other hand, friction property of CNx in N$_2$ with humidity 50%, in air with humidity 25% and 50% showed ca. 0.11, 0.14 and 0.14, respectively. Friction property of a-C in dry N$_2$, in N$_2$ with humidity 50%, in air with humidity 25% and 50% showed ca. 0.09, 0.15, 0.14 and 0.14, respectively. It was found that humidity increase both friction coefficients of CNx and a-C. It was observed that the thickness of transfer layer formed on Si$_3$N$_4$ ball decreased with humidity. The average physical adsorption structure of 6H$_2$O on sp$^2$-carbon containing nitrogen shows in Fig. 2. By hydrogen bonding, hydrogen atom of H$_2$O was close to carbon atom of sp$^2$-carbon. The distances showed 2.10 Å and 2.86 Å compared to 3.35 Å of sp$^2$-carbon interlayer distance. The physical adsorption of H$_2$O on the sp$^2$-carbon structure shows chemically strong bond compared to sp$^2$-carbon interlayer structure. It is suggested that the physical adsorption structure of H$_2$O in environmental gas with the humidity causes the decrease of thickness of transfer layer. By the decrease of thickness of transfer layer, both friction of CNx and a-C increased with humidity.

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REFERENCES