Influence of Nitrogen on Friction Properties of CN_x Coatings Based on First-Principles Molecular Dynamics and Tight-Binding Quantum Chemical Molecular Dynamics Methods

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1. Introduction

Carbon nitride (CN_x) and diamond like carbon (DLC) films are expected as solid lubricants for MEMS and have been studied actively. For previous experiments, CN_x and DLC films showed low friction properties, and it is pointed out that chemical reactions strongly influence their friction properties. CN_x film is expected to have lower friction properties and more durable than DLC film. However, this mechanism has not been clarified well. This is because it is very difficult to obtain atomic-scale dynamics directly during the chemical reactions by experiments, which affect their friction properties. In this study, our purpose is to clarify the super-low friction mechanisms of hydrogen terminated CN_x (H-CN_x) film compared to hydrogen terminated DLC (H-DLC) in an atomic scale by our first-principles molecular dynamics (FPMD) and tight-binding quantum chemical molecular dynamics (TB-QCMD) methods.

2. Method

We employ our TB-QCMD code, Colors, and FPMD code, Violet, for performing friction simulations of the H-CN_x and H-DLC coatings. In H-CN_x model, 15% of carbon atoms are replaced by nitrogen atoms. The upper substrate is slid with 100 m/s and the bottom atoms of the lower substrate are fixed. A load is given to the upper substrate in a direction vertical to the interface. We calculate the cumulative averaged friction coefficient defined as the following equation; $\mu = F_x/F_z$. Here, F_x and F_z represent the sums of horizontal and perpendicular forces to the upper substrate, respectively. All simulations are performed at 300 K.

3. Results and discussion

First, to investigate super-low friction mechanism of CN_x films, we performed friction simulations of H-CN_x/H-CN_x and H-DLC/H-DLC films by our TB-QCMD method. Fig. 1 shows time variation of the friction coefficients of the films under 1 GPa and 5 GPa. In Fig. 1 (a), both H-CN_x/H-CN_x and H-DLC/H-DLC films take a low friction coefficient of 0.05 under 1 GPa. Here, our previous study presented that the generation of C-C bonds at the interface of DLC film caused a rise of the friction coefficient [1]. Since C-C and C-N bonds are not generated at the interfaces of these films under 1 GPa as shown in Fig. 1 (a), the friction coefficient keeps a low value during the friction. In Fig. 1 (b), H-CN_x film shows a low friction coefficient of 0.07 under 5 GPa. On the other hand, H-DLC film shows a high friction coefficient of 0.43 under 5 GPa. Here, while C-C and C-N bonds are not generated at the interface of H-CN_x film, many C-C bonds are generated at the interface of H-DLC film. Thus, we suggest that H-CN_x film has more stable and lower friction properties than H-DLC film under high pressure condition because of preventing the generation of C-C bonds. The details of these results are discussed in the conference.

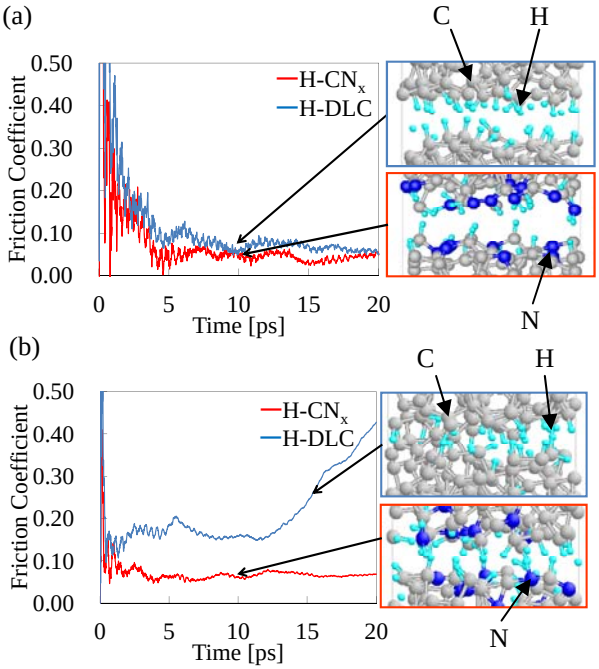

Fig. 1 Time variation of the friction coefficients of H-CN_x and H-DLC under (a) 1 GPa and (b) 5 GPa.

4. References

[1] Hayashi, K., Sato, S., Kubo, M. et al., "Fate of methanol molecule sandwiched between hydrogen-terminated diamond-like carbon films by tribochemical reactions: tight-binding quantum chemical molecular dynamics study", Faraday Discuss., 156, 2012, 137-146.