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Study on Superlow Friction Mechanism of Diamond-like Carbon Film using Non equilibrium Molecular Dynamics Simulation

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【Introduction】 Diamond like carbon (DLC) is often used as a tribo-coating due to its excellent properties, i.e. hardness, wear resistance and chemical stability. It can also provide a superlow friction state to the friction system with some specific lubricants and additives. Although many researchers have studied a friction performance of DLC coating using experimental techniques, a detailed friction reduction and superlow friction mechanism has not yet been unveiled. In the present study, we investigated an atomistic friction mechanism of DLC film using non equilibrium molecular dynamic simulation.

【Method】 We used our developed MD code "NEW-RYUDO-CR"[1], which can deal with chemical reaction dynamics, to study the DLC friction. In the code, the chemical reaction is stochastically considered, thus realizing chemical reaction dynamics for a large complex system within much less computation cost.

【Results】 In the first stage of this study, we investigated a friction mechanism of DLC against itself using the superimposed model of two constructed DLC substrates as shown in Fig 1(a). The MD simulation was performed for 500,000 steps with time step of 1.0 fs. To simulate the friction, the external pressure of 1 GPa was applied to the top surface of the substrate while it forcedly slid with horizontal velocity of 10 m/s. The resultant friction coefficient was 0.60 which was calculated from the force acting on the sliding carbon atom divided by normal load. This value is quite reasonable for a vacuum dry friction. Fig. 1(b) shows the interface structure at the simulation time of 120 ps, and we can see the C-C covalent bond formation between two substrates. This would inhibit the smooth sliding of two solid surfaces. Subsequently, by introducing several H atoms into the constructed model, the hydrogenated DLC (H-DLC) was built, and the similar MD simulation was performed for this model. As the result, the friction coefficient was 0.001 and we could not observe any chemical bonding on the contact surface (Fig. 1(c)). This is due to no covalent interaction between two surfaces. Hence, the results suggest that the chemical bonds in sliding interface potentially affect friction properties in nature. Further details will be discussed in the presentation.

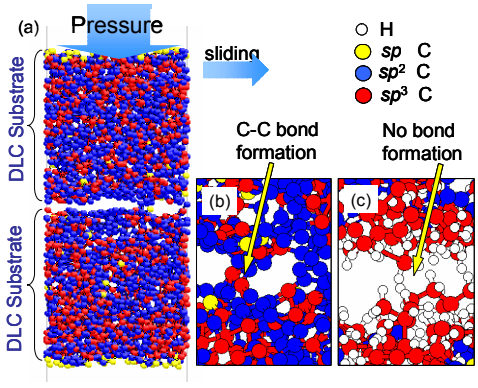

Figure 1(a) DLC friction model, structure of (b) DLC/DLC and (c) H-DLC/H-DLC interfaces.

1) Y. Morita et al., *Appl. Surf. Sci.*, **254** (2008) 7618.