TRIBO-CHEMISTRY OF DIAMOND (111) IN CONTACT WITH WATER

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KEYWORDS
Diamond Coatings; Humid Environments; Quantum-Mechanical Molecular Dynamics

ABSTRACT
Ultralow friction of diamond in humid environments is of both scientific and industrial interest [1]. Experimental groups suggested that the surface passivation by H and OH groups plays an important role in ultralow friction of diamond [2]. Zilibotti *et al*. [3] showed that water molecules undergo chemical reactions with a diamond (001) surface under a high normal pressure by Car-Parrinello molecular dynamics (MD). However, due to their high computational cost, the accessible time scale is still limited to a few picoseconds. Since running-in processes and related phase transitions occur on larger time scales, little is known about the steady-state atomic-scale friction mechanisms of water-lubricated diamond surfaces.

We here present the mechanism underlying the ultralow friction of a diamond (111) surface in contact with water molecules using the density-functional tight-binding (DFTB) MD method [4]. To understand the effects of the relative humidity on the friction of diamond, we perform sliding simulations of non-reconstructed diamond (111) surfaces interacting with different numbers *n* of water molecules. Simulations are carried out by rigidly moving the upper surfaces for 0.1 ns at a constant velocity of 100 ms^{-1} under an average normal pressure of 5 GPa. Figure 1a shows the friction coefficient as a function of *n*. The presence of a small amount of water initially induces cold welding and amorphization resulting in high friction. However, during running-in a tribo-induced Pandey reconstruction emerges preventing the diamond surfaces from cold welding, thus leading to ultralow friction (Fig. 1b). When the amount of water increases further, diamond surfaces are sufficiently passivated with H and OH groups. The surface passivation occurs via the two reaction mechanisms: (i) the dissociative chemisorption of a water molecule and (ii) Grotthuss-type proton transport [5]. The sliding of H/OH-passivated surfaces also leads to stable and ultralow friction (μ = 0.02). Our models provide microscopic insight into the kinetics at diamond/water interfaces and explain the experimentally observed ultralow friction of diamond at a wide range of relative humidity.

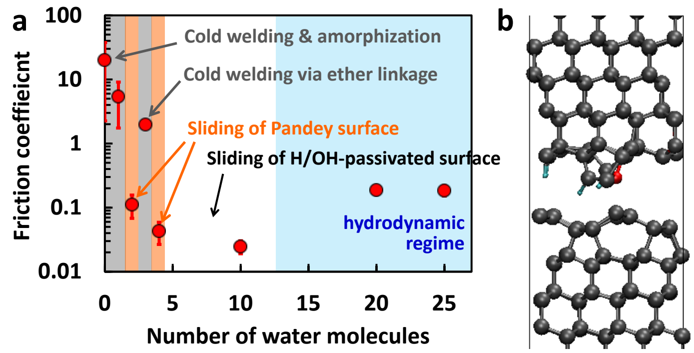

Fig. 1 (a) Friction coefficient as a function of the number of water molecules. (b) Representative example of the tribo-induced Pandey reconstruction.

ACKNOWLEDGMENTS
T.K. acknowledges financial support by JSPS Overseas Research Fellowships. Simulations were carried out on the supercomputer JURECA at the Jülich Supercomputing Center.

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