Controlling friction in carbon and ceramic systems by mechano-chemistry

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The increasing demand for sustainable tribology has accelerated the development of environmentally friendly lubrication solutions such as water-related lubricants in combination with carbon or ceramic surfaces under boundary lubrication conditions. Atomistic simulations reveal superlubricity mechanisms for glycerol-lubricated tetrahedral amorphous carbon (ta-C) [1] and Si_3N_4 [2]. In our quantum molecular dynamics (MD) simulations glycerol concurrently chemisorb on both tribopartners and bridge the tribogap. Sliding-induced mechanical strain triggers complete fragmentation of the lubricant. In the case of ta-C surfaces, superlubric graphenoid passivation layer forms. For Si_3N_4 surfaces, glycerol's oxygen reacts with Si to silica, while the carbon forms superlubric disordered graphene-nitrides. Both results are supported by experiments.

Keywords: atomistic simulations, tribochemistry, superlubricity, tribo-material

1. Introduction

Minimisation of frictional energy losses and wear is one basic prerequisite for sustainable mobility. For instance, reducing friction in passenger cars to ultra- ($0.1 \geq \mu \geq 0.01$, μ: friction coefficient) and superlow ($\mu \leq 0.01$) levels would significantly lower fuel consumption and global CO_2 emission. Carbon and ceramic coatings in combination with water-based fluids are important candidates for future suprasliding bearings. However, the mechanisms are hardly understood.

2. Methods

We perform density functional based tight-binding (DFTB) MD of sliding ta-C/ta-C and Si_3N_4/Si_3N_4 surfaces under glycerol boundary lubrication.

3. Results

We perform sliding simulations of glycerol-lubricated ta-C and find a complete mechano-chemical fragmentation of the glycerol followed by the formation of graphenoid surface passivations (Fig. 1a,c). This leads to superlubricty of the tribosystem (Fig. 1b).

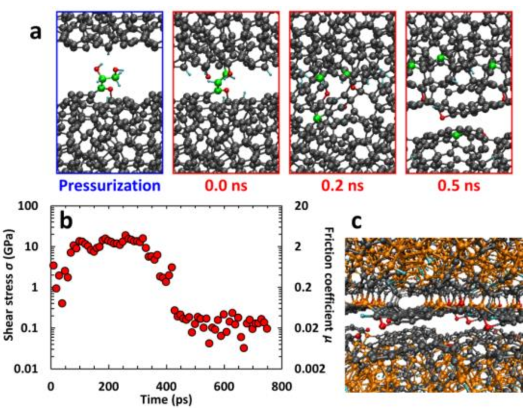

Figure 1: DFTB-MD of ta-C lubricated by glycerol.

Superlubricity in Si_3N_4 boundary lubricated by glycerol can be explained by mechano-chemical decomposition of glycerol and subsequent formation of disordered graphenoid CN layers (Fig. 2). Here, sliding favors the formation of Si-O and of C-N bonds – the precursors of silica and carbo-nitride phases (Fig. 2a).

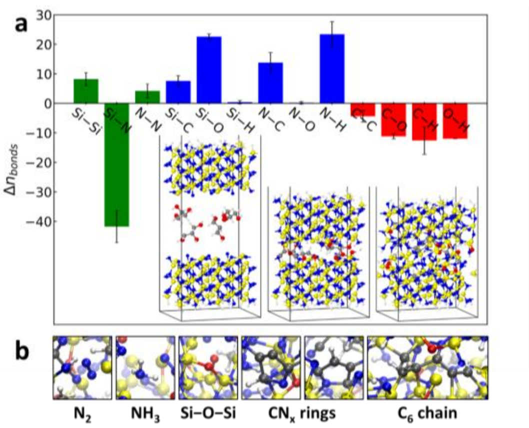

Figure 1: Superlow friction of Si3N4 tribopairs.

4. Outlook

At the end of the talk tribochemical wear of hard ta-C boundary lubricated by ZDDP will be elucidated by DFTB-MD simulations [3].

5. References

[1] T. Kuwahara et al., Mechano-chemical decomposition of organic friction modifiers with multiple reactive centres induces superlubricity of ta-C, **Nature Communications** 10, 151 (2019)

[2] Y.Long, et al. In situ synthesis of graphene nitride nanolayers on glycerol-lubricated Si3N4 surfaces leads to superlubricity, **ACS Applied Nano Materials** (2020)

[3] V.R.Salinas Ruiz et al. Interplay of mechanics and chemistry governs wear of diamond-like carbon coatings interacting with ZDDP-additivated lubricants (2021)