MECHANO-CHEMICAL DECOMPOSITION OF ORGANIC FRICTION MODIFIERS WITH MULTIPLE REACTIVE CENTRES INDUCES SUPERLUBRICITY OF ta-C

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Superlubricity of tetrahedral amorphous carbon (ta-C) coatings under boundary lubrication with organic friction modifiers is important for industrial applications, but the underlying mechanisms remain elusive. Here, combined experiments and simulations unveil a universal tribochemical mechanism leading to superlubricity of ta-C/ta-C tribopairs [1]. Pin-on-disc sliding experiments show that ultra- and superlow friction with negligible wear can be achieved by lubrication with unsaturated fatty acids or glycerol, but not with saturated fatty acids and hydrocarbons. Atomistic simulations reveal that, due to the simultaneous presence of two reactive centers (carboxylic group and C=C double bond), unsaturated fatty acids can concurrently chemisorb on both ta-C surfaces and bridge the tribogap. Sliding-induced mechanical strain triggers a cascade of molecular fragmentation reactions releasing passivating hydroxyl, keto, epoxy, hydrogen and olefinic groups. Similarly, glycerol's three hydroxyl groups react simultaneously with both ta-C surfaces, causing the molecule's complete mechano-chemical fragmentation and formation of aromatic passivation layers with superlow friction (Fig. 1).

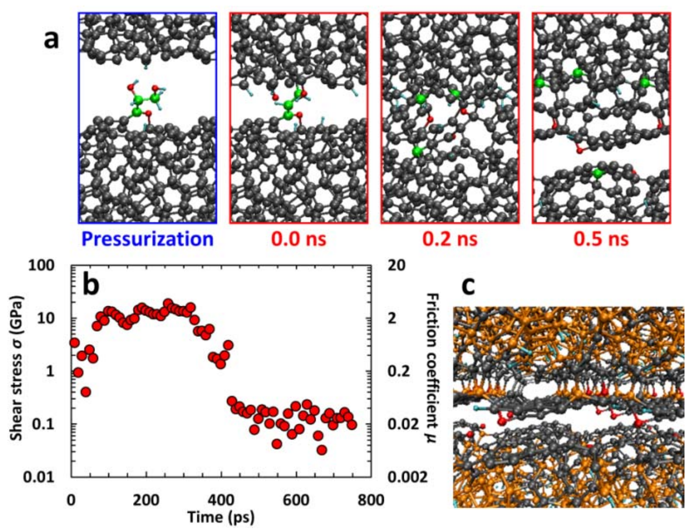

Figure 1: A QMD simulation of two ta-C surfaces lubricated with a glycerol molecule. (a) Snapshots of the 1-ns sliding simulation. (b) Evolution of the shear stress *σ* and friction coefficient *μ*. (c) Shear-induced aromatic passivation of both ta-C surfaces. 3- and 4-fold coordinated C atoms are represented in grey and orange spheres, respectively.

REFERENCES

[1] T. Kuwahara, P.A. Romero, S. Makowski, V. Weihnacht, G. Moras, M. Moseler, Mechano-chemical decomposition of organic friction modifiers with multiple reactive centres induces superlubricity of ta-C, Nature Communications **10**, 151 (2019)