DRY FRICTION OF AMORPHOUS CARBON ON EPITAXIAL GRAPHENE: INSIGHTS AND OBSERVATIONS

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ABSTRACT
Epitaxial graphene on SiC(0001) exhibits superlow friction due to its weak out-of-plane interactions. Friction force microscopy experiments conducted with silicon and diamond tips reveal a sharp escalation in friction, increasing by one order of magnitude beyond a threshold normal force. Density-functional tight-binding simulations conducted on silica interacting with epitaxial graphene propose that this high-friction regime, devoid of wear, involves intermittent sp^3 rehybridization of graphene under contact pressures exceeding 10 GPa. Additionally, the simultaneous formation of covalent bonds with the silica tip's surface and the underlying SiC interface layer introduces a third mechanism that constrains the superlow friction observed on epitaxial graphene, complementing dissipation in elastic instabilities and wear processes [1]. In this study, we investigated the sliding behavior of aromatic and H/OH-terminated amorphous carbon (a-C) on the graphene/ SiC(0001) system at 300 K. The study is divided into two distinct phases. The initial phase involves the utilization of Density-Functional Tight-Binding (DFTB) simulations to explore friction regimes under varying pressures, encompassing both low pressure (ranging from 5 to 15 GPa) and high pressure (ranging from 17.5 to 30 GPa) conditions. In the subsequent phase, classical Molecular Dynamics (MD) simulations were conducted to scrutinize the super-low sliding regime, extending up to 100 nN (equivalent to 3.5 GPa), employing a non-reactive force field.

Our DFTB results show that, at low pressures (up to 20 GPa) during the 200 ps simulation, there are no reactions between a-C and the underlying graphene, resulting in smooth sliding behavior. Initially, the shearing plane is located between a-C and graphene. However, as pressure increases (from 17.5 GPa to 20 GPa), significant changes occur. Within the first 30 ps, the two graphene layers bond, and inner a-C atoms form bonds with graphene. As the simulation progresses, hydrogen atoms break bonds with a-C and form new ones with graphene, partially passivating it. This shift in behavior is reflected in the velocity gradients, transitioning from being situated between graphene layers to being between a-C and the graphene layer. At higher pressures (>30 GPa), graphene begins amorphizing within the first few picoseconds of the simulation.

Classical MD simulations are faster than DFTB simulations, enabling us to mimic experimental scales using a 20 nm a-C tip. Molecular statics precisely replicate slow tip movements, incrementally displaced in 0.2 Å steps for indentation and scratching. Simulations covered pressures from 20 nN to 100 nN (1.9 GPa to 3.3 GPa) with results based on 30 Å indentation. The results indicate that aromatic and H-terminated tips display exceptionally low friction, approaching zero, consistent with experimental friction forces for normal loads ranging from 10-100 nN. In contrast, H/OH-terminated tips exhibit higher friction levels, ranging from 0.66 to 0.81 nN, incompatible with experimental observations. These findings highlight the significant impact of termination groups on friction characteristics.

REFERENCES
[1] B. Szczefanowicz et al., Formation of intermittent covalent bonds at high contact pressure limits super-low friction on epitaxial graphene, Phys. Rev. Research 5, L012049 (2023).