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Tuning Hysteretic Friction Behavior of Supported Atomically Thin Nanofilm Via Substrate Roughness

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Abstract

The hysteretic friction behavior of supported atomically thin nanofilms with varied underlying substrate roughness was studied using atomic force microscopy (AFM) experiments and molecular dynamics (MD) simulations. Substrates with different roughness were prepared by immersing silica in KOH solutions of varying concentrations for different durations, and their roughness was measured and characterized on different scales using AFM and white-light interferometry. Graphene and MoS_2 were exfoliated onto silicon wafers with varied underlying substrate roughness. Tapping mode confirmed that the degree of interfacial contact between the nanofilms and the substrates varied with substrate roughness, with smoother substrates exhibiting better adhesion. In the friction experiments, two diverging friction hysteretic behaviors were found during the loading–unloading cycle: one showed positive hysteresis, i.e., friction forces that were higher during unloading than during loading, and the other showed negative hysteresis, where the friction forces were lower during unloading than during loading. Experimental observations revealed that as the substrate roughness decreased, the friction hysteresis transitioned from positive to negative, although the critical roughness at which the transition occurred differed for the two nanofilm thicknesses. MD simulations were conducted on a rough silicon substrate with varied roughness, reproducing the diverging friction hysteretic behaviors. The simulations revealed that a high roughness results in poor contact between graphene and the substrate, creating a weak interface that causes positive friction hysteresis because the pucker generated in the nanofilm during unloading cannot recover promptly. As the roughness decreases, improved contact leads to a strong interface, resulting in the opposite hysteresis. Furthermore, MD simulations highlighted the influence of nanofilm thickness; namely, thicker films require a lower substrate roughness to achieve better adhesion, which also explains why MoS_2 with twice the thickness exhibits the friction hysteresis transition later than graphene. The essential role of the underlying substrate roughness in the 2D nanofilm/substrate system revealed in this paper provides a mechanism for tuning the friction behaviors of supported 2D materials.