2D or not 2D? How Nanoscale Surface Roughness Impacts the Frictional Properties of Graphene and MoS_2

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Control of friction and wear is a ubiquitous challenge in numerous machined interfaces ranging from biomedical implants, to engines, to nano- and micro-scaled devices, with the energy losses associated with friction and wear having significant impacts on the economies of the world. Notably, the combined energy losses and the associated system downtime for maintenance of machines due to friction and wear, contribute to an estimated loss of ~$200 billion/year in the United States alone.[1,2] As such, developing new approaches for the control of friction at interfaces is a critical need. One of the key challenges in developing boundary lubrication schemes for such systems, is how to reduce friction and wear at the rough surfaces typical of machined interfaces, where nanoscaled asperities of ~ 10 – 20 nm rms roughness, dominate the interfacial contacts. The robust mechanical properties of two-dimensional (2D) nanomaterials has made them of significant interest for modifying surface frictional properties. It has been found that many 2D materials can readily adapt to surface structure on the atomic scale however, when deposited on substrates with nanoscopic roughness, a conformal coating cannot be fully formed due to competition between adhesion to the nanoscopic asperities of the substrate and the corresponding bending strain of the material. This often leaves a mixture of supported (bonded) and unsupported regions which respond differently to applied load. To investigate this in detail, we have developed a model platform to study friction in true nanoscaled asperity-asperity contacts using silica nanoparticles to form substrates with asperities of controlled radius of curvature (*ca.* 3 – 35 nm), matching those found in many machined interfaces. Here we describe a combination of AFM structural, nanomechanical and confocal Raman spectroscopic studies of graphene and MoS_2 on silica surfaces with controlled nanoscopic roughness, to examine the how surface roughness impacts their frictional properties. Additionally, as noted above, since substrate adhesion is a critical factor in the control of friction at these interfaces, we have also explored how the deposition of self-assembled monolayers (SAMs) of alkylsilanes with varying terminal functional groups (e.g. $–NH_2$, $-CH_3$, $-C_6H_6$) on the substrates also influence the corresponding structure, and the adhesion and friction in these 2D nanomaterials, when deposited on top of the SAM layers. The ability to tune and control roughness in these materials on the nanoscale also has other implications in the applications of these materials in electronics and catalysis.

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[2] Jost, H. P.: Tribology micro & macro economics: A road to economic savings. *Tribology & Lubrication Technology* **2005**, *61*, 18-22.

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