MORPHOLOGY-DEPENDENT FRICTION OF ADSORPTION FILMS: MOLECULAR DYNAMICS OF SDS AND CTAB AT THE H_2O | AU(111) INTERFACE

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ABSTRACT
In solution, amphiphilic surfactants aggregate on immersed surfaces. The resulting physisorbed film exhibits morphology-dependent boundary lubrication behavior, in particular with respect to the static and kinetic friction coefficient in the stick-slip regime [1]. In order to illuminate this interdependence of morphology and friction on the nanoscopic scale, our present work focuses on two model surfactants of broad application in industry and science: the anionic sodium dodecyl sulfate (SDS) and the cationic cetyltrimethylammonium bromide (CTAB), at idealized water–gold interfaces. We utilize existing SDS and CTAB parametrizations to conduct numerical atomic force microscopy (AFM) and friction force microscopy (FFM) experiments by means of classical all-atom molecular dynamics (MD).

Adsorption films and their nanotribological properties are typically characterized by AFM probing. Such measurements yield topographic profiles, but the conclusion upon a film's underlying structure is not straightforward and oftentimes debated: Are observed patches actually mono-, bi- or multilayers? Are stripes to be interpreted as hemicylinders or cylinders? In our sample case of SDS and CTAB on Au(111), both surfactants are known to form flat-lying monolayers at low concentrations. With increasing surface coverage, stripe-like aggregates assemble. These are of hemicylindrical nature in the case of SDS [2], whereas CTAB has been argued to form full cylinders [3]. At these concentration regimes, equilibrium MD of postulated film aggregates do not necessarily distinguish physical from non-physical configurations: Fig. 1 shows both (b) dense monolayers as well as (c) cylindrical aggregates of CTAB to behave metastable throughout MD-typical time scales. Thus, we map out force-distance curves on AFM probe approach towards substrates covered with different film morphologies across a range of concentrations as well as anisotropic lateral forces felt by an FFM probe tangentially sliding on these films. Contrasted against the response in experimental reality, we investigate how such measurements might help to discriminate between competing interpretations of AFM measurements.

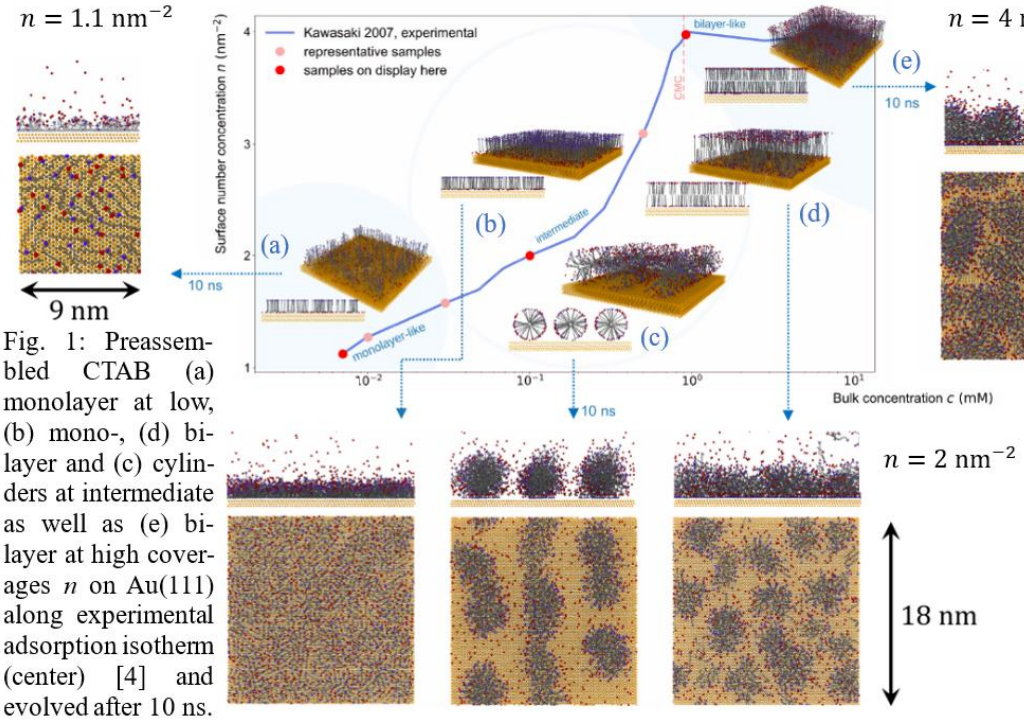

Fig. 1: Preassembled CTAB (a) monolayer at low, (b) mono-, (d) bilayer and (c) cylinders at intermediate as well as (e) bilayer at high coverages n on Au(111) along experimental adsorption isotherm (center) [4] and evolved after 10 ns.

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