Novel Lubrication Schemes for Silicon-Based Microelectromechanical Devices

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Molecular dynamics simulations are used to study the adhesion and friction between nanoconfined self-assembled monolayers (SAMs) composed of fluorinated chains and mixed fluorinated/hydrogenated chains on silica. Fluorinated materials are known to exhibit low critical surface tension and high thermal and mechanical stability. While fluorinated SAM coatings are more stable against elevated temperature and humidity than hydrocarbon silane monolayers, they are known to be less effective as lubricants on smooth silicon surfaces than hydrocarbon SAMs. The likely reason for the weaker performance is that the perfluorinated monolayer is not as well-ordered as the hydrocarbon SAM due to their van der Waals diameter being larger than the distance between the active sites on the SiO2 surface. The concept of mixed monolayers composed of hydrocarbon and fluorocarbon chains could enable the formation of well-ordered perfluorinated SAMs on silica. The frictional behavior of pure and mixed hydrocarbon/fluorcarbon SAMs is investigated as a function of normal load, shear velocity, and chemical composition of the SAM coating.