Molecular Simulation Studies of Nano-Scale Friction

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Nonequilibrium molecular dynamics simulations were performed to study nano-scale friction between two Si(111) surfaces covered with alkyl monolayers immersed in liquid solvents (Figure 1). Three pairs of interfaces, ranging from hydrophobic CH_3/CH_3 to hydrophilic OH/OH, were studied. Three solvents, including water, methanol, and *n*-decane were used to represent different solvent polarities. A fundamental understanding of nano-scale friction at different interfaces in various solvents is very important to micro- or nanoelectromechanical systems (MEMS/NEMS), particularly, bio-MEMS/NEMS.

Tip-based hybrid molecular simulations were performed to study the frictional properties of alkanethiol self-assembled monolayers (SAMs) on Au(111) at the atomic /frictional force microscopy (AFM/FFM) experimental time scale (Figure 2). Various parameters influencing frictional properties were investigated, including chain length, terminal group, scan direction, and scan velocity. In addition, the application of the hybrid molecular simulation technique will be demonstrated for studies of the unbinding pathways of molecular pairs at the experimental time scale.

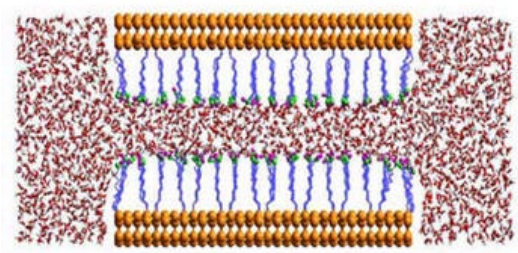

Figure 1. Non-equilibrium molecular dynamics simulations of nano-scale friction between two Si(111) surfaces covered with OH terminated alkyl monolayers immersed in water.

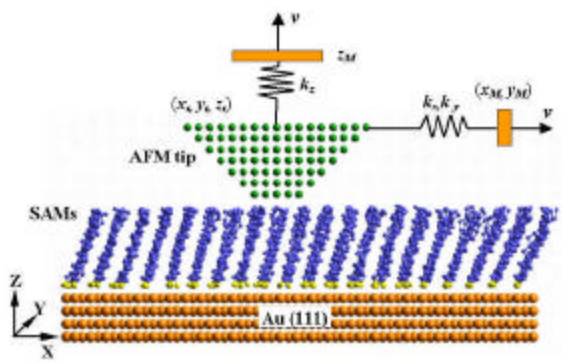

Figure 2. Tip-based hybrid molecular simulations of the nano-scale frictional properties of self-assembled monolayers on Au(111) at the AFM/FFM experimental time scale.