Molecular Dynamics Studies of Friction in Alkylsilane and Hydroxyalkylsilane Coated MEMs Devices

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The adhesion and friction properties of the native amorphous silicon oxide layer in silicon-based micro- and nano-electromechanical devices (MEMS/NEMS) have a strong influence on device control, performance and durability. To improve the friction and adhesion properties surfaces coated with alkylsilanes have been proposed and shown to reduce the friction forces as the chain length of the alkylsilanes increases. In an effort to develop surfaces with varying surface energy that can be used in lubrication systems in which a bound lubricant (i.e., alkylsilane) is combined with a mobile layer, alkylsilanes with hydroxyl terminal groups have also been studied. At low normal loads, the friction force of surfaces coated with hydroxylalkylsilanes are higher than the corresponding surfaces coated with akylsilanes, but surfaces coated with hydroxyalkylsilanes show a maximum as a function of normal loads.

We use molecular dynamics simulations to study the friction forces of silica surfaces coated with alkylsilanes, hydroxyalkylsilanes and their mixtures. The systems of interest have been studied over a wide range of normal loads. In agreement with previous studies, friction forces for the surfaces coated with hydroxyalkylsilanes are one order of magnitude higher than surfaces coated with alkylsilanes. We also find the maximum reported for the surfaces coated hydroxyalkylsilanes, but also find that this is a local maximum, after which, the friction forces behave normally and the friction and normal forces are linearly dependent. The surfaces coated with mixtures of alkylsilanes and hydroxyalkylsilanes show a friction behavior dependent on the composition of the surfaces. The friction forces increase linearly as the composition changes from the pure alkylsilane to the pure hydroxyalkylsilane.