Development of Novel Bound + Mobile Lubrication Strategies for Aerospace Applications

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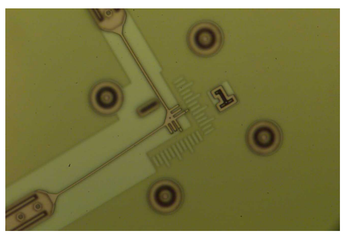
Abstract

Lifetimes of moving interfaces can often be extended by using a thin lubricant coating. However, most lubricants have reasonably narrow conditions of temperature and pressure over which they provide effective protection against friction and wear. This is unacceptable for many aerospace applications, which continually travel between drastically different environments. To gain new insights into the nanoscale properties of monolayer lubricants, we are carrying out both quartz crystal microbalance experiments and atomistic computer simulations. Using these techniques we have explored the effectiveness of lubricants, amount of mobile phase needed, transport properties of the mobile phase, and incorporation mechanisms into defected sites. These together help us move towards a better understanding of novel lubricants for aerospace applications.

Motivation

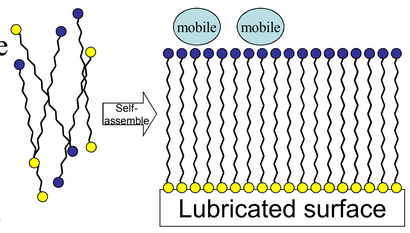
- New lubricants are needed for aerospace applications that can operate at both terrestrial conditions (high humidity + ~20 °C) and space conditions (vacuum, +/ ~100's °C).



- Micro-Electro-Mechanical Systems (MEMS) devices are both **test beds** for new lubrication strategies and potentially important **components of air/space craft.**

- One **proposed solution** would be to use a two phase lubrication scheme, such as a bound + mobile scheme

- The first phase would initially coat and protect the surface and the second phase would replenish the coat in-situ when damaged during use

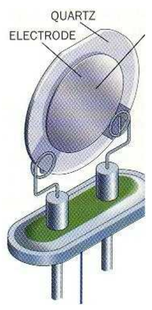


Experimental Equipment

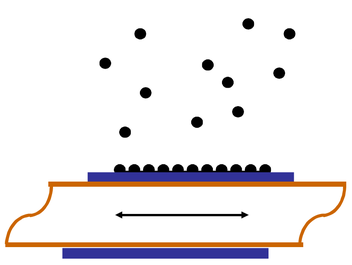
- The quartz crystal microbalance (QCM) is used to characterize the tribilogical properties of adsorbed monolayers

- The isolated QCM oscillates in shear mode at a characteristic and well defined frequency

- Presence of adsorbed molecules lowers the resonant frequency



$$f_{ads} = (4f_{res}^2/Zq)(m/A)$$



- If the shear stress is below about 10^3 N/m^2, it will "slip" enough to be detected by the QCM:

$$\delta(Q^{-1}) \propto \delta(A^{-1})$$

$$\delta(Q^{-1}) = 4\pi\tau\delta f_{\circ}$$

- The slip time is deduced from Q and f

Molecular Dynamics Simulations

Molecular Dynamics Simulations

- MD simulations provide an atomic view of the time evolution of complex material systems and processes
- Empirical potentials are used to determine the forces acting on the atoms in the system
- These forces are then used to integrate Newton's equations of motion to determine the acceleration, velocity, and position for all atoms in the system

QCM study of Bound + Mobile lubricants

Objective

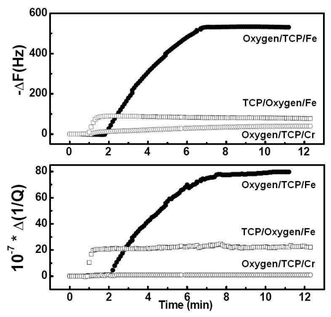
- Using a QCM to measure frequency and amplitude of bound plus mobile lubricant
- The amount of the adsorbed species can be determined by measuring the frequency
- Measurements of amplitude change can be used to calculate "slip", which is used to determine how good of a lubricant the adsorbed layer is

Summary of Findings

- TCP and TBPP both adsorb on the surface and slip, indicating that they are possible lubricants
- PFTS in combination with ethanol is found to lubricate to a certain point but too much ethanol can be detrimental due to a build up of capillarity forces

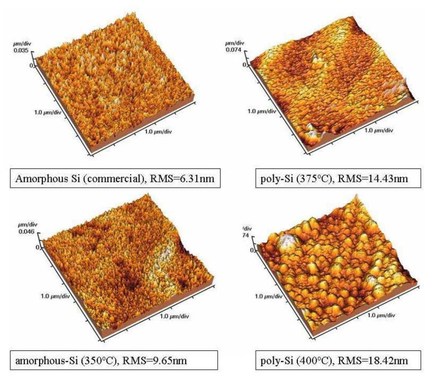
Background

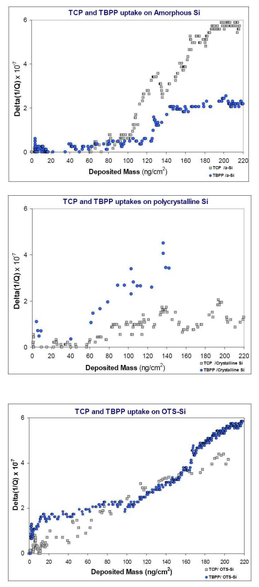
- Previous studies of TCP in the presence of oxygen and two metal substrates indicated:
  1) If the adsorbed layer "slipped" at all it was a **successful** macroscale lubricant
  2) If no slip was measured then the layer was a **poor** macroscale lubricant



Results

Bound + Mobile: Si/ODTS + TCP/TBPP





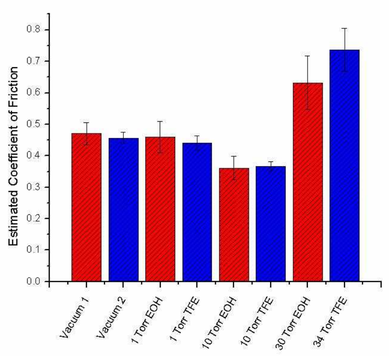
- Uptake and slip times were measured on a variety of substrates
- The OTS was deposited on the amorphous Si substrate
- It can be seen that the TCP and TBPP readily adsorb on the Si/OTS system

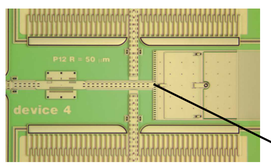
Vapor Phase Lubricant	Polycrystalline silicon		Ozone-cleaned amorphouse silicon		Si+OTS	
	Film thickness (monolayer)	Slip time τ (ns)	Film thickness (monolayer)	Slip time τ (ns)	Film thickness (monolayer)	Slip time τ (ns)
TCP	5	0.14	5	0.90	5	0.48
TBPP	3	0.25	5	0.30	5	0.24

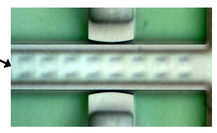
- TCP and TBPP are found to slip when deposited on all of these substrates
- This indicates that the gas phase mobile lubricant would protect the device with and without the bound SAM

Bound + Mobile: Si/PFTS + Alcohol

- Addition of small partial pressures of alcohol reduces the static engineering coefficient of friction possibly due to a decrease in the force of adhesion
- Partial pressures above 50% reduces performance due to a build up of capillariy forces







Pinch contact

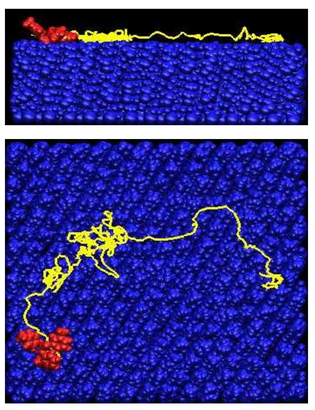
Molecular dynamic simulations of Bound + Mobile lubricants

Objective

- For the Bound + Mobile scheme to be successful the transport and incorporation of mobile layer into damaged/defected sites needs to be understood
- Molecular dynamics simulations are used to *understand* diffusion and incorporation mechanisms and to the *calculate* the transport coefficients, activation energies, and energy barriers

Summary of Findings

- We find the adsorbed molecule sits on top of a tightly packed SAM and diffuses rapidly across the surface, high rates allow mobile species to quickly reach damaged areas
- To incorporate into the defect a molecule has to overcome an anisotropic energy barrier, which results from SAM tilt
- Once inside the defect the mobile species becomes localized with drastically different dynamics than on the ideal terrace, indicating it's preferential location to be at the defect wall
- Addition of step edges changes the dynamics of the surface diffusion, as step size is increased diffusion takes place by hops at the side wall

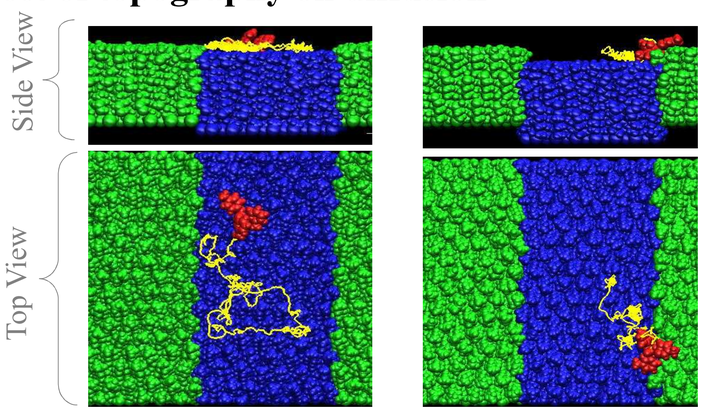


Results

Ideally flat SAM

- The TCP molecule stays on top of the OTS SAM
- Diffusion takes place through a series of hops and tumbles
- No preferential orientation of TCP with the substrate is found
- A low activation barrier of 9 kJ/mol is calculated for this system

Effect of topography on diffusion

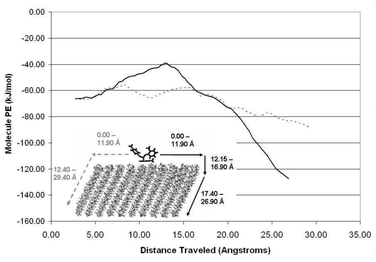


Step of 2.54 Angstroms

Step of 5.08 Angstroms

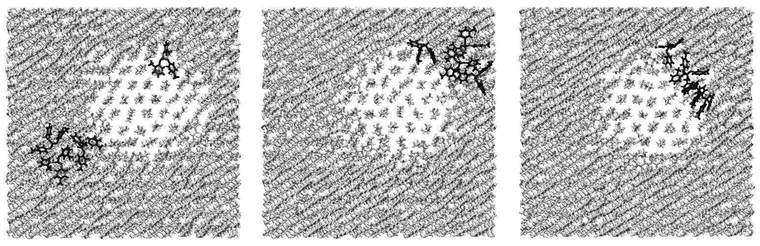
- Preliminary results show differences in diffusion for systems with steps
- Small steps lead to directional diffusion, while large steps lead to slower transport rates

Incorporation into defects



Irving and Brenner, JPCB (2006)

- Molecules adsorbed in the defect behave in a different fashion then those on the terrace
- They become localized and almost stationary as they attempt to embed in the OTS sidewall to maximize coordination
- To incorporate molecules have to go over an *anisotropic energy barrier*



- Defects and voids are inevitable in processing and use.
- They provide sites of strong, preferential, adsorption at these sites
- Molecules adsorbed at defect sites could be one reason they "slip" less than on amorphous Si