Nanotechnology with Emphasis on Tribology:
A Combined Experimental and Simulation Study
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Principal Investigator
Peter T Cummings (ptc@utk.edu)
University of Tennessee and Oak Ridge National Laboratory

Co-Principal Investigators
Steve Granick, University of Illinois
Hank Cochran, Oak Ridge National Laboartory
Shengting Cui, University of Tennessee
Gary Grest, Sandia National Laboratory

The moving contact of two solid surfaces results in friction and wear. Lubrication is necessary to reduce damage and to enable reliable operation. Fundamentally the phenomena of friction, wear, and lubrication involve molecular mechanisms occurring on a nanometer scale, and a good understanding of lubricant behavior on the this scale is thus of primary importance to developing new technology for reduction of loss due to friction. Practical examples are many; one in particular occurs in magnetic recording devices such as computer hard disks, where lubrication of the surface of the recording media is essential to insure smooth operation and durability. The economic value involved is enormous: the magnetic recording industry alone is currently estimated to have an annual worldwide market about $100 billion.

In addition to disk drives, devices with moving parts separated by only nanometers are increasing in their technological and economic importance. Myriad novel microelectromechanical systems, such as micro-motors, are under development. Fluid between the moving surfaces in such devices is subjected to extremely high rates of shear strain, 10^8 s^{-1} or higher, more than an order of magnitude higher than previously attained in controlled experiment. Often, lubrication is essential to the practical use of such devices, and the US data storage industry has identified developing new lubricants and surface finish as one of six major technical objectives to achieving increased recording density and read/write speed.

In this project, a multidisciplinary, multi-institutional collaboration is undertaking a fundamental study of lubrication at nanometer scale, including experiments with Granick's surface rheometer instrument and non-equilibrium molecular dynamics simulation, a technical scope beyond the capabilities of any one of the participants. A major goal of this project is to achieve overlap in shear rate between experiments and simulations on the same systems. A second goal is to extend both expermental and computational study to more complicated systems and surface characteristics, including surfaces with chemical and topographical heterogeneity, that are of primary technological importance. A third goal is to study not only the steady-state shear response of nanotribology systems but also their transient behavior, including the technologically important issues related to adhesion. A final, but overarching, goal of the proposed work is to seek new methods to reduce the friction and wear of moving

surfaces separated by only nanometers. These goals are being pursued through coordinated experiments and calculations that probe the fundamental phenomena involved at a molecular level.

The primary experimental tool is Granick's surface rheometer. Prior to this project, the highest accessible strain rates on this instrument were about 10^5 s^{-1}. Our hope was to extend the strain rate capabilities of our instrument to ca. 10^8 s^{-1} by raising the resonant frequency of the piezoelectric bimorphs which drive the shear by up to two orders of magnitude beyond the ca. 300 Hz frequencies employed at the start of the project. While this has been achieved, the resulting measurements of shear stress and viscosity are not reliable due to exfoliation of the mica sheets at such high shear rates. Hence, it is becoming clear that reliable experimental characterization at very high strain rates may be very difficult to achieve.

The prime reason for pushing the experiment to very high strain rates is that the simulations of nanoconfined lubricants must be performed at very high strain rates (typically ca. 10^{10} s^{-1} and higher). The reason for needing very high strain rates in simulation is that the small system sizes (typically the number of molecules N is of the order of $10^3 - 10^6$) in simulations result in thermal noise being a significant factor (unlike the case in a macroscopic system, since the thermal noise is proportional to N^{-1}). Hence, in order to distinguish the measured rheological properties from the thermal noise background, the simulations must be run at high strain rate. In order to access low strain rates, we must simulate much larger systems, preferably for long periods of time (in excess of 10 ns). Our goal was to reduce the strain rate attained in simulations to ca. 10^7 s^{-1} (overlapping experiment by ca. an order of magnitude). We have achieved this by a combination of brute force (longer, larger simulations on parallel supercomputers) as well as performing the simulations in a different way – by applying a constant shear stress and measuring the induced velocity profile rather than applying a velocity field and measuring the shear stress. This has enabled us to access strain rates around $10^7 - 10^8$ s^{-1}.
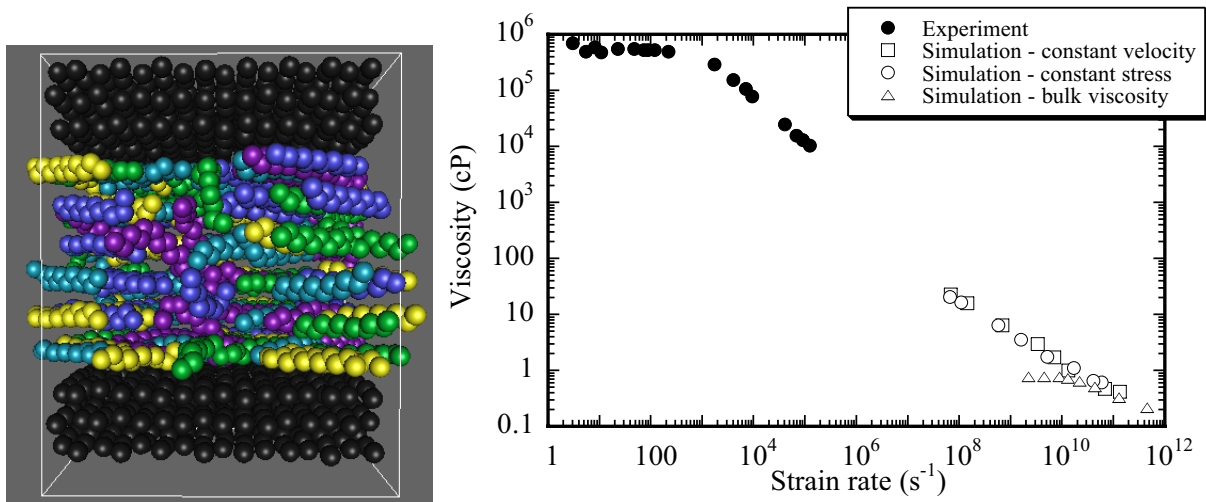
Simulations and experiments have been performed on dodecane confined between mica sheets. We show above on the left a snapshot from the simulation for mica sheets separated by six layers of dodecane. The viscosity measured in these simulations is compared with experiments performed as part of this project in the graph on the right. The simulation were performed both at constant velocity of moving mica surfaces and at constant stress applied to

the mica surfaces, and the results are seen to be consistent. Also shown is the strain rate dependent viscosity for bulk dodecane at the same conditions (ambient temperature and pressure). Clearly, the transition between Newtonian (strain rate independent viscosity) and non-Newtonian behavior (strain rate dependent viscosity) behavior takes place in the bulk at a strain rate of order 10^{10} s^{-1}, while for the nanoconfined dodecane, the transition is at around 10^3 s^{-1}. Additionally, the Newtonian viscosity of the confined dodecane is five orders of magnitude higher than that of bulk dodecane.