Dynamics of Organic Films on Different Time Scales

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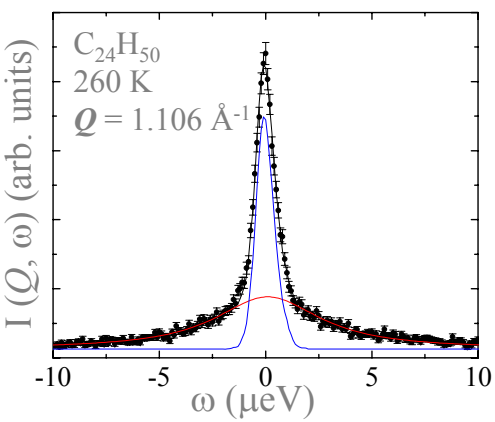
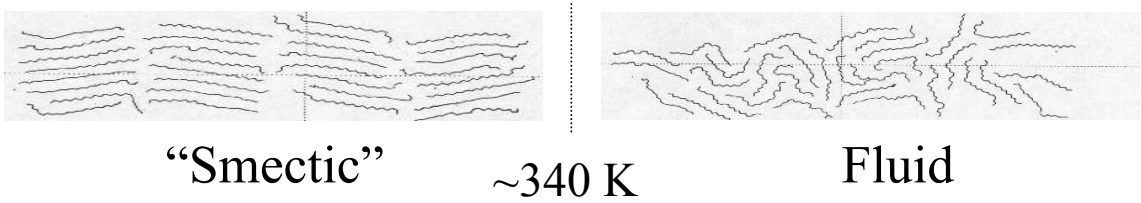
Alkane molecules are the principal constituents of commercial lubricants. They are also one of the building blocks of the lipid molecules that form cell walls. More generally, they serve as prototypes of complex polymers used in coatings, adhesives, and electronic devices. We have recently investigated the diffusive motion of alkane molecules in ultra-thin films adsorbed on solid surfaces using neutron scattering with very high energy resolution (a millionth of an electron volt). Using computer simulations of the molecular dynamics to interpret the neutron spectra, we are able to probe the random motion of the alkane molecules on a nanosecond time scale. Such studies contribute to the understanding of cell membrane elastic properties and may eventually lead to the design of better lubricants.



Typical quasielastic neutron spectrum from an alkane film taken on the High Flux Backscattering Spectrometer at the Center for Neutron Research, National Institute of Standards and Technology.



Top view of the computer simulation cell looking down on two different alkane monolayer phases: a liquid-crystal-like phase (left) and a fluid phase (right).

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Alkanes (chemical formula C_nH_{2n+2}) are flexible chain-like molecules that are of general interest in materials science as prototypes of more complex polymers used in coatings, adhesives, and electronic devices. They are also of interest in their own right as the principal constituents of commercial lubricants. In the area of biological physics, alkanes play an important role as building blocks of lipid molecules in the membranes that form cell walls. A microscopic understanding of the structure and dynamics of very thin alkane films could potentially lead to significant advances in a variety of polymer-based technologies as well as improve our understanding of cell membranes.

Over the past five years, we have been successful in using synchrotron x-ray scattering to elucidate the structure and growth mode of solid alkane films adsorbed on solid substrates. These substrates include silver single crystals (which model metal surfaces of interest in lubrication applications and metal contacts used in electronic devices) as well as single-crystal silicon wafers used in the semiconductor industry.

By combining neutron diffraction measurements and molecular dynamics simulations, we have demonstrated that the melting transition in an alkane monolayer adsorbed on a graphite surface is qualitatively similar to the well-known gel-to-fluid transition in bilayer lipid membranes in which intrachain and lattice melting occur simultaneously. An alkane film, consisting of a single layer of molecules without headgroups, thus provides a simpler system than a membrane for a detailed study of the molecular dynamics through the melting transition. More recently, we have used neutron scattering with very high-energy-resolution (neutron energy transfers down to one millionth of an electron volt) and molecular dynamics simulations to investigate the changes in molecular conformation (shape) occurring in the alkane monolayer on a nanosecond time scale. Such experiments complement nuclear magnetic resonance studies by probing the length scales relevant to the diffusive conformational motion. They also suggest the type of measurement which can be performed on real lipid membranes using the new neutron spectrometers that will be available at the Spallation Neutron Source when it is completed at Oak Ridge National Laboratory in 2006. This work was published in the January 30, 2004 issue of Physical Review Letters.

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Education:
An undergraduate student (Matthew Simpson), two graduate students (Armand Diama and Haiding Mo), and a postdoctoral research associate (Sven Trogisch) contributed to this work. Matthew Simpson participated in an Undergraduate Research Mentorship Program in summer 2003 and is now taking research courses with the PI. He is an A+ student in physics and math who plans to pursue a combined physics Ph.D./M.D. program. Haiding Mo received his Ph.D. in 2004 and is presently a postdoc working with Pulak Dutta in the Department of Physics at Northwestern University. Armand Diama is still a member of the PIs' group and is performing related experiments. Sven Trogisch has accepted an industrial research position in Dresden, Germany.

Undergraduate research:
In the video clip, undergraduate student Matt Simpson and postdoc Sven Trogisch are shown conducting measurements with an Atomic Force Microscope on an alkane film coating a silicon wafer used in electronic device fabrication.