# 518i Surface Morphology and Interfacial Properties of Lubricant Nanofilms

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The structure of nanofilms, which plays a critical role in determining their dynamics and performance, is of great technical interest in polymer science. Molecularly thin lubricant film, *e.g.*, perfluoropolyether (PFPE), which has been widely employed to protect and lubricate the head-disk interface (HDI) of information storage devices, is one of the successful industrial applications of nanoscale oligomeric fluid systems. As a key component of the integrated HDI design, surface morphology of lubricant films, which is directly related to the film surface tension, indirectly influences the mechanical stability of the flying read/write head.

Commercially available PFPEs contain a chemical structure of $X\text{-}[(OCF_2\text{-}CF_2)_p\text{-}(OCF_2)_q]\text{-}OX$ ($p/q \approx 2/3$). Here, the endgroup X is $CF_3$ (nonfunctional) for Z and $CF_2CH_2OH$ (functional) for Zdol, where the hydroxyl groups induce additional interactions due to hydrogen or dangling bonds [1]. The interaction between the PFPE and the substrate (*e.g.*, carbon overcoat) is another important factor in determining the film surface morphologies [2]. Via scanning microellipsometry, as the PFPE films are spread on silica and carbon surfaces, "dewetting" has been observed only for Zdol while Z films does not exhibit this phenomenon [3].

Here, molecular dynamics (MD) simulations based upon the coarse-grained, bead-spring model via the Langevin equation, were performed to generate the equilibrated surface morphologies, where the dependences on the molecular architecture (*e.g.*, molecular weight and endgroup functionality) and film thickness (*e.g.*, sub/mono/multi-layers) were also included. From the 3D molecular structural visualization, we have observed that Z films always exhibit a smooth surface; however, Zdol film starts to "dewet" as soon as it exceeds monolayer but recovers its smoothness as it reaches three layers. In addition to the conventional surface characterization methods, *e.g.*, average film height and root-mean-square (RMS) roughness, we introduced a new technique, the wavelet transform, into the surface analysis, which typically decomposes the given surface morphology into several frequency/wavelength components and is especially good for surfaces containing non-stationary signals, *e.g.*, sharp discontinuity. By correlating the surface morphology parameters (*e.g.*, wavelet entropy) with the transport properties (*e.g.*, self-diffusion coefficient), a strong correlation between the equilibrium nanostructure and surface dynamics was revealed, where each transition point corresponds to a specific structural change occurring inside the film, *e.g.*, percolation threshold.

Further, a quasi-equilibrium MD simulation was carried out to demonstrate our "thought experiment" of nano mechanics, *e.g.*, compression and tension. Initially, PFPE films were "coated" onto two nanoscale separated solid surface facing each other. As the top surface moves downward, a complete contact of nanofilms occurs, which is so called "compression." As the top surface moves upward at a constant speed, molecules are elongated to form the fluid bridge between the two surfaces, which is known as "tension". A hysteresis loop in the film normal stress profile was observed for the first time, indicating the existence of PFPE viscoelasticity. Furthermore, the film surface tension, which highly depends on endgroup functionality as well as film thickness, was further extracted from simulated "compression" mechanics to provide a thermodynamic criterion for the film uniformity/stability.

[Reference]

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