Study of Nanotribological Behavior of a Perfluoropolyether Coating on Diamond-like-carbon Film by Molecular Dynamics Simulations

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Molecular dynamics simulations of a multilayer sliding system, a perfluoropolyether film sandwiched between two diamond-like-carbon films, are carried out to investigate atomic level frictional mechanisms. Results show that the competition of adhesion strength at the two interfaces determines the solidified lube to slide as either stick-slip or dynamic manner. The friction force is generated both from the surface adhesion and the normal loading. With concurrent effects from material stiffness, normal loading and surface roughness, we found the formation of heterogeneous stress distributions at close contact regions along the interface when the normal loading is either very low (<10MPa) or very high (>500MPa). Meanwhile, the fluctuation of friction force is inversely proportional to the normal loading. Using a half-spherical shaped slider, the interfacial contacting area can be described by the Johnson-Kendall-Roberts model when the normal loading is large enough to induce significant deformations on the lube film. Otherwise, the frictional mechanics is largely dependent on atomic adhesion, where strong fluctuated friction force is observed.

Keywords: friction, nanotribology, molecular dynamics, PFPE, mechanics, interface.