Lubricated Normal and Sliding Contact of Fractal Rough Surfaces at the Atomic Scale

Solhjoo, Soheil; Vakis, Antonis I.

The International Conference on Understanding and Controlling Nano and Mesoscale Friction: June 22-26 2015, Istanbul, Turkey

LUBRICATED NORMAL AND SLIDING CONTACT OF FRACTAL ROUGH SURFACES AT THE ATOMIC SCALE

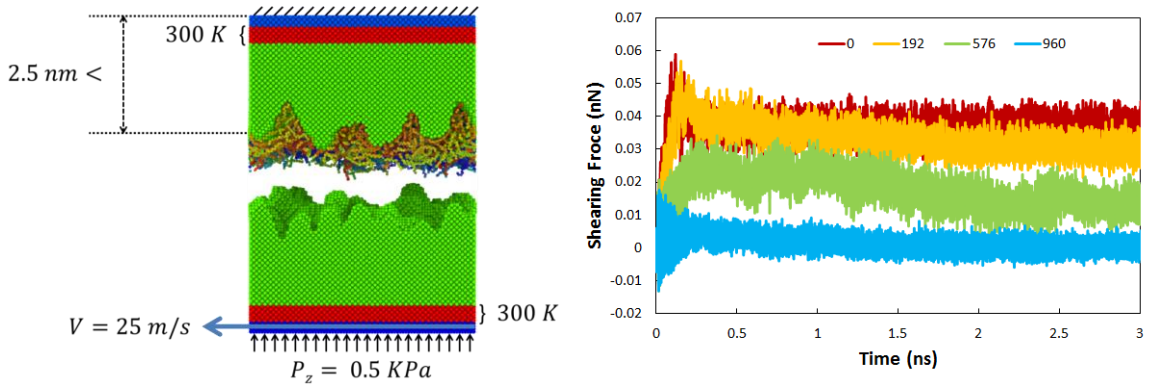
Soheil Solhjoo, Antonis I. Vakis

Advanced Production Engineering, ENTEG-FMNS, University of Groningen, The Netherlands

The friction of contacting interfaces is a function of surface roughness and applied normal load. Moreover, in the case of lubricated contact, frictional behavior changes with lubricant film viscosity and density. Many atomistic studies of rough contacts adopt simplified sinusoidal shapes for the roughness, and model the interface as that between a deformable surface and a rigid flat; however, sinusoidal corrugation is most often a non-physical representation of roughness which is fractal in nature. In this work, three-dimensional contacts between atomically, randomly rough fractal surfaces of nickel lubricated with different volumes of n-hexadecane molecules were simulated via the molecular dynamics method using LAMMPS [1].

A pair of fractal surfaces [2] was numerically generated with an RMS roughness and correlation length of 10 Å and 8 Å, respectively. These were used to construct two atomic blocks of fcc-nickel (see figure), with each block divided into three layers: rigid, thermostatic, and free deformable. An embedded-atom-method (EAM) potential [3] was applied to nickel atoms. Different numbers of hexadecane molecules (0, 192, 576, and 960) formed a lubricant film, and were modeled via the TraPPE-UA [4,5] and Lennard-Jones potentials. Finally, the radial density function (RDF) of nickel atoms was used to define contact at the interface.

Results showed that increasing the lubricant volume reduced the solid-solid contact area during normal contact, and also diminished the changes in the surface RMS roughness, suggesting that the lubricant could provide sufficient bearing support at the interface. Moreover, during the sliding process, the lubricant volume affected the shearing force, which decreased with increasing lubricant volume (see figure). Similarly, increasing film coverage (dependent on lubricant volume) was also found to reduce the contact interference between the solid surfaces.



The atomistic system setup (left), and the reduction in shearing force with increasing lubricant volume during sliding (right).

[1] Plimpton, S., 1995, J. Comp. Phys., 117, 1.

[2] Garcia, N., Stoll, E., 1984, Phys. Rev. Lett., 52, 1798.

[3] Zhou, X.W., Johnson, R.A., Wadley, H.N.G., 2004, Phys. Rev. B., 69, 144113.

[4] Martin, M.G., Siepmann, J.K., 1998, J. Phys. Chem. B., 102, 2569.

[5] Pàmies, J.C. et al., 2003, Mol. Simul., 29, 463.