Friction Coefficients and Mechanisms of MoS2 Nanoparticles from Molecular Dynamics Simulations

H.J Cian[1], C.H. Yu[1], and C.S. David Chen[1]

[1] Department of Civil Engineering, National Taiwan University, Taipei, Taiwan.

*Corresponding author: dchen@ntu.edu.tw

We studied friction coefficients and mechanisms of MoS2 nanoparticles from molecular dynamics simulations. A covalent bond potential of molybdenum and sulfur were implemented in LAMMPS and tri-layered capsular structured MoS2 nanoparticles subjected to different amplitudes of normal stress were performed. We found average friction coefficient about 0.05 and lower friction coefficients for higher normal stresses, both observations agreed well with experimental measurements. In addition, when the underlying mechanisms switched from sliding to rolling, significant reduction (about 50%) of friction coefficients was observed.

Keywords: Nano friction, MoS2, lubrication, MD