

Friction dynamics in soft-bio and polymeric systems

ABSTRACT:

Amontons' classical law of friction states that the resistive force against the motion of a sliding macroscopic object on a surface is proportional to the applied external normal force. Recent advances in nanotribology and single-molecule experiments have revealed that at nanoscopic scales, conventional laws do not apply due to the adhesive forces and thermal fluctuations, and these laws should be reviewed. To shed light on the friction of soft-materials in single molecule level, the friction of laterally pulled single peptides over various substrates are put under investigation in the presence of water using extended Molecular Dynamics (MD) simulations and the stochastic Fokker-Planck equation. We also discuss the friction experienced by a peptide in a peptide bundle as a function of a confinement parameter, which is the number of neighbouring chains in the bundle. We show that the friction of hydrogen-bonded matter obeys a simple equation in the biologically relevant low-velocity viscous regime.

In addition, we conducted MD simulations for various polymer brush systems where multiple polymer chains are grafted on a surface. In this simulations two polymer brushes are pressed towards each other and slid past each other at a prescribed inter-plate distance and velocity. We observed that friction of brush systems is of similar behavior to that found in single bio-molecular systems: The friction exhibits both linear (viscous) and non-linear regimes depending on the driving velocities. Our findings are also consistent with proposed scaling arguments. We also observe that the topology of the grafted chains, i.e., whether they are linear or ring chains, can affect the friction dynamics.