COMPUTATIONAL MODELING IN NANOMETER-SCALE TRIBOLOGY

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Tribology is the science about friction. Friction and wear have long been recognized as limiting factors to numerous applications and many areas of technology. Thus, there has been significant interest in understanding and controlling these processes. Some historical examples include the ancient Egyptians, who invented new technologies to move the stones used to build the pyramids; Coulomb, whose studies of friction were motivated by the need to move ships easily and without wear from land to the water; and Johnson, whose study of automobile windshield wipers led to a better understanding of contact mechanics and surface energies. Today, research and development is focused on microscale and nanoscale machines with moving parts, which continue to challenge our fundamental understanding of friction and wear. This has motivated researchers to study friction on ever-smaller scales to determine its fundamental cause. The study of atomic-scale friction has also paved the way for new innovations, such as the development of self-lubricating surfaces and wear-resistant materials. The mechanisms that lead to friction at the atomic scale can sometimes be quite distinct from the mechanisms that dominate at the macroscale. This has implications for nanometer-regime devices such as magnetic storage disks, which have been shrinking in size steadily over the last few years, and microelectromechanical systems where atomic-scale friction, adhesion and wear are the dominant processes.

The scientific study of atomic-scale friction has been on the rise since the late 1980's. This is due to the simultaneous development of sophisticated new experimental tools to measure friction over nanometer-scale distances at low loads, the rapid increase in computer power and processing speed, and the maturation of theoretical methods needed to study material processes in a realistic manner. For example, the surface force apparatus has provided new information related to friction and lubrication for many liquid and solid systems with unprecedented resolution. The friction-force and atomic-force microscopes allow the frictional properties of solids to be characterized with atomic-scale resolution under single asperity contact conditions. Other methods, such as the quartz crystal microbalance, also can be used to provide insight into the origin of friction. With the experimental apparatus currently available, it is possible to study sliding surfaces at the atomic-scale, and ultimately relate observed behavior to macroscopically-observed phenomena.

Theoretical models and simulations assist in the interpretation of experimental data and provide predictions of phenomena that the experiments can subsequently confirm or refute. These include analytic models and large-scale molecular dynamics (MD) simulations, among others. Analytic models have long been used to study friction. The strength of these idealized models is that they can be used to divide the complex motions that create friction into basic components defined by quantities such as spring constants, the curvature and magnitude of potential wells, and bulk phonon frequencies. The main weakness of these approaches is that simplifying assumptions must be made to apply these models to study friction that may lead to incorrect results.

Molecular dynamics computer simulations represent a compromise between analytic models and experimental conditions. For instance, MD simulations rely on approximate interatomic forces and classical dynamics, which is similar to what is needed for analytic models. In addition, simulations can reveal unanticipated phenomena that require further exploration, which is similar to what occurs in experiments. Moreover, a poor choice of simulation conditions can result in meaningless result, which is also the case in experimental studies. Thus, a thorough understanding of the strengths and weaknesses of MD simulations is crucial to both successfully implementing this approach and understanding its results.

Atomistic computer simulations appear, on the surface, to be rather straightforward to carry out: given a set of initial conditions and a way of describing interatomic forces, one simply integrates Newton's classical equation of motion using one of several standard methods. The simulations yield new relative atomic positions, velocities and forces and the atomic responses can be followed using animated movies. However, the effective use of MD simulations to study atomic-scale friction requires an understanding of many details not apparent in this simple analysis.

MD simulations of molecularly thin water film confined between two atomically flat diamond plates are described in the present work. The TIP4P rigid model is used for water molecules. Crystalline or glassy order is induced across the film when high pressure is applied. The onset of the glassy phase is characterized by rapidly increasing relaxation times. These manifest themselves through changes in the diffusion constant.

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