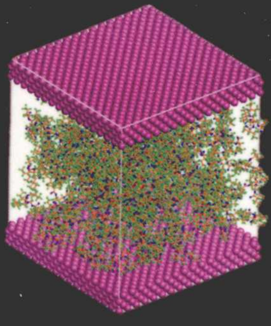
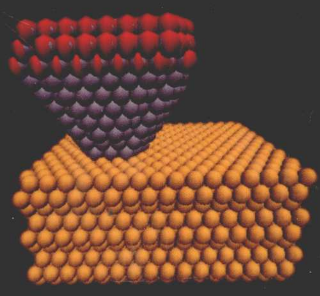
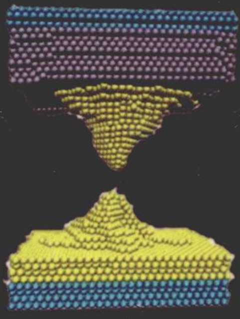
MICRO- and NANOSCALE PHENOMENA in TRIBOLOGY

Edited by
Yip-Wah Chung

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Preface

Whether dealing with large bearings and gears in a wind turbine or microscale components inside a digital projector, successful operations of these macro- and microdevices depend on understanding and controlling interactions occurring at the micro and the nano scales. This is a field that has benefited a great deal from multidisciplinary collaborations, as evidenced by the numerous international conferences and symposia on the subject over the past twenty years. It is with this spirit that we put together this monograph, which is the result of a short course presented by the National Science Foundation (NSF) Summer Institute on Nanomechanics, Nanomaterials, and Micro/Nanomanufacturing, held in San Diego, California, in April 2010. I hope this monograph represents not a collection of isolated subjects, but a tapestry of the convergence of the multiple science and engineering disciplines and the bridging from the macro to the micro world.

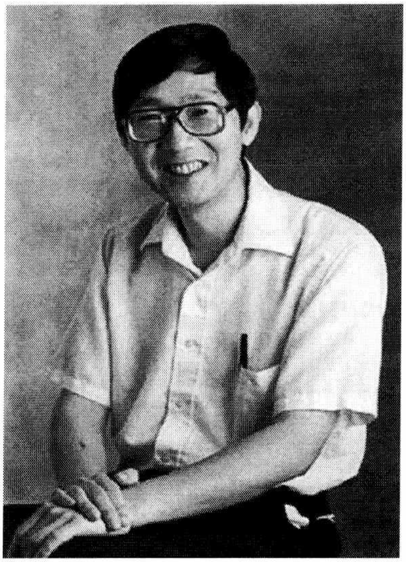
The monograph begins with a short narrative on the evolution of tribology in the micro and nano world. Chapter 2 describes the range of contact conditions spanning the gap between macroscale and nanoscale contacts. Then a primer on macroscale sliding phenomena and how these relate to interfacial film formation and friction performance is presented, followed by a review of instrumentations for examination of microscale sliding contacts. Chapter 3 presents an overview of fundamental continuum treatments of interfacial contact and lubrication under a wide range of conditions, including recent advances in contact simulation. Given the large surface-to-volume ratio in nanoscale materials, structures, and devices, surface forces are destined to be dominant. Chapter 4 gives a thorough account of the nature of surface energies and forces in these structures, as well as adhesion in dry and wet environments. This sets the stage for the next two chapters. Chapter 5 describes how one performs friction measurements at the nano scale and how such friction data can be interpreted, sometimes within the framework of continuum mechanics. Given that magnitudes of surface forces and friction can be modulated by surface topography, Chapter 6 begins with a discussion of various experimental techniques to fabricate micro- and nanotextured surfaces. This is followed by a comprehensive series of results demonstrating how such textures affect adhesion, friction, and wetting.

Tribological properties are affected not only by the surface topography, but also by the environment. Chapter 7 emphasizes the importance of surface chemistry in tribology and reviews some of the environmental effects reported for various tribological interfaces of metals, ceramics, coatings, and solid lubricants. The chapter also presents an in-depth discussion of the effects of alcohol and water vapor on capillary adhesion, friction, and wear of silicon oxide surfaces, followed by examples where environmental effects can be used to mitigate friction and wear. Chapter 8, the final chapter, is on molecular dynamics simulation, from the basic question of what it is and what it can do for tribology, to examples where molecular dynamics simulation has made significant contributions, and to investigations to extend the length and time scales of simulation.

This monograph project is the culmination of efforts of many friends and colleagues. I wish to express my sincere thanks to all the authors for their hard work and cooperation to make this monograph a reality: Allison Shatkin, Jennifer Ahringer, and Andrea Dale of Taylor and Francis for overseeing the publication details, Dr. Ken Chong and Dr. Clark Cooper of the National Science Foundation for their continuing support of the Summer Institute, and Alpana Ranade of Northwestern University for the logistical support of the short course.

Yip-Wah Chung
Northwestern University
March 2011

Editor Biography



Yip-Wah Chung obtained his PhD in physics from the University of California at Berkeley. He joined Northwestern University in 1977. He is currently professor of materials science and engineering and mechanical engineering at Northwestern. His research interests are in surface science, tribology, thin films, and alloy design. He was named Fellow, ASM International; Fellow, AVS; and Fellow, Society of Tribologists and Lubrication Engineers. His other awards include the Ralph A. Teetor Engineering Educator Award from SAE, the Innovative Research Award and Best Paper Award from the ASME Tribology Division, the Technical Achievement Award from the National Storage Industry Consortium (now the Information Storage Industry Consortium), the Bronze Bauhinia Star from the Hong Kong Special Administrative Government, and the Advisory Professor from Fudan University. Dr. Chung served two years as program officer in surface engineering and materials design at the National Science Foundation. His most recent research activities are in infrared reflecting coatings, low-friction surfaces, strong and tough coatings, and high-performance alloys. His favorite hobbies are photography and recreational flying. He holds several FAA ratings, including commercial multiengine instrument, instrument ground instructor, and advanced ground instructor.

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1 Introduction

Yip-Wah Chung

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1.1 HISTORY

Tribology, the study of friction, wear, and lubrication has become a multidisciplinary endeavor. Historically, mechanical engineering was the home of tribology. Much of the early studies were focused on contact stresses, lubricant film thickness, flash temperatures, and wear modeling, mostly in powertrain and manufacturing components. In lubricated contacts, one can minimize wear by operating under conditions where two sliding surfaces are separated by a lubricant film, with thickness at least three times that of the composite surface roughness to ensure full separation. This is known as the *full-film* or *hydrodynamic lubrication* regime. However, whether driven by economics or the nature of technology never satisfied to be left alone, the performance of mechanical systems continues to be pushed to higher levels—higher loads, higher temperatures, smaller form factors, and lighter structures. As a result, sliding interfaces no longer have the luxury of being separated by a full lubricant film, and direct contact between surfaces often occurs.

The importance of surface composition and testing environment in controlling friction and wear became clear to Don Buckley of the National Aeronautics and Space Administration (NASA) in the 1960s (Buckley 1968a, b). He performed fundamental tribological studies using surface analytical techniques and in situ friction measurements under well-defined environmental conditions. Buckley is truly the pioneer of his time, demonstrating the close interaction between surface science and tribology. Unfortunately, most surface scientists during that period were focusing their attention more on semiconductor surfaces and catalysis than tribology. It wasn't until 1991 that the first tribology symposium was held outside traditional tribology societies. The American Chemical Society organized its first symposium on tribology (Surface Science Investigations in Tribology), involving international speakers from universities, industry, and government laboratories (Chung, Homola, and Street 1992). This symposium brought together researchers from chemistry, chemical engineering, materials science, mechanical engineering, and physics to talk about different aspects of tribology. To the best of my knowledge, this is also the first symposium in which molecular dynamics simulation studies in tribology were presented. This marks the beginning of many such interdisciplinary symposia hosted by the American Chemical Society, American Society of Mechanical Engineers, American Vacuum Society, the Society of Tribologists and Lubrication Engineers, and others.

1.2 IMPACT OF TRIBOLOGY

In the ensuing twenty years, the tribology community has witnessed the convergence of surface science, development of new micro- and nanoscale diagnostic techniques, invention of novel materials, coatings, and lubricants, and demand for higher operating efficiencies and durability in machineries large and small. We have made great strides in improving machine efficiency and durability. An excellent example is the internal combustion engine. Back in the 1970s, one cubic inch of engine displacement on average produced 0.5 hp, and the recommended oil change interval was 3,000 miles. Today, there is no shortage of internal combustion engines giving more than 1.5 hp per cubic inch of engine displacement, and oil change is typically at 5,000-mile intervals or greater. Powertrain and drivetrain components are now much more reliable than before. Passenger cars lasting more than 100,000 miles are now considered more a norm than a rarity.

While tribology cannot claim credit for all the advances of the internal combustion engine and other devices, there have been many numbers cited for the significant economic benefits of proper application and practice of tribology, in the range of a few percent of gross domestic product (GDP). Regardless, benefits of having a reliable piece of tribological hardware go beyond dollars and cents. A crashed hard drive or a stalled car may entail some inconvenience and frustration, but a prematurely worn orthopedic implant can affect someone's health and quality of life. In some instances, a failed piece of tribological hardware can have fatal consequences. Nothing illustrates this better than Alaska Airlines Flight 261, which crashed in the Pacific Ocean on January 31, 2000, about 40 miles west of Malibu, California. All 88 people onboard perished. According to the National Transportation Safety Board report (Aircraft Accident Report NTSB/AAR-02/01), the probable cause of this fatal accident was due to "a loss of airplane pitch control resulting from the in-flight failure of the horizontal stabilizer trim system jackscrew assembly's acme nut threads. The thread failure was caused by *excessive wear* resulting from Alaska Airlines' *insufficient lubrication* of the jackscrew assembly" (emphases added). This is a sober reminder that tribological failure can and will affect people's lives in profound ways.

1.3 THE WAY FORWARD

While performance improvements of conventional machineries can be achieved by evolutionary changes of existing materials, technologies, and practices, the same cannot be said for conventional machineries subjected to more demanding operating conditions, or new mechanical devices that operate under entirely different length scale regimes. In the former situation, one may be dealing with some combination of high flash temperature and high contact stress in a chemically reactive environment, such as may occur in today's advanced high-power-density drivetrain and powertrain components. The most notable examples of the latter are computer disk drives and microelectromechanical systems (MEMS). In these instances, tribological interactions between surfaces depend on phenomena happening at the micro- and nanoscale. In both situations, bulk properties and continuum mechanics alone are no longer adequate to fully describe these interactions. This could be the result of dynamic material transfer from one surface to another, micro- and nanoscale roughness influencing capillary condensation and lubrication, surface chemical reactions, surface forces controlling adhesion, and so on. With the advanced experimental techniques available today, we can study these mechanical and surface chemical phenomena with high degrees of precision, including buried interfaces in some cases. We now have powerful molecular dynamics techniques to simulate micro- and nanoscale tribological phenomena over reasonable length and time scales, providing us with insights and details not accessible before.

Researchers from physical and biological sciences, various disciplines of engineering, and medicine are now working on different aspects of tribology. The success and future of tribology must rely on collaborative efforts across traditional boundaries to gain better understanding of the fundamental micro- and nanoscale interactions, and to apply such knowledge to the design and fabrication of durable tribological components for engineering and biological systems. More than ever, tribology will play a critical role in our quest for a sustainable future, whether by increasing energy efficiency of mechanical systems, enhancing reliability of powertrain systems subjected to frequent start-stops associated with hybrid vehicles, or designing new bearing and gear surfaces for durable wind-turbine operations. The tribology community has much to contribute for a better world!

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2 Macroscale to Microscale Tribology
Bridging the Gap

Kathryn J. Wahl

CONTENTS

2.1 INTRODUCTION

The past quarter century has brought many changes in our ability to simulate, create, and delicately probe surfaces and structures at ever decreasing scales. Experimentalists have learned to create complex nanostructures, perform ever finer lithography, and pattern single monolayers of graphene. Ultrathin and small structures are readily investigated by tools such as scanning tunneling microscopy (STM) and atomic force microscopy (AFM), which have matured into a broad array of nanoscale surface characterization and imaging techniques widely available on user-friendly commercial platforms. Similarly, these advances provide big opportunities and changes to the field of tribology. Now, nearly every laboratory is equipped with tools that can examine interfaces having contact widths of atomic dimensions with sub-nN force resolution. Where once it was a challenge for molecular dynamics simulations to include a single atom defect in a lattice, modern simulations include thousands of atoms, incorporate amorphous materials, and combine atomic and continuum modeling to tackle larger systems. We now have broad capabilities to examine sliding contacts and adhesion over scales spanning many orders of magnitude, down to the single asperity level.

The focus of this chapter is to treat the topic of experimental tribology, specifically with the aim of examining *what* microscale processes occur in sliding contacts and *how* they impact friction processes. At the macroscopic scale, contacting interfaces are large enough (many microns to mm wide) that we can often literally see what processes are taking place during sliding. At smaller scales, we use the term *microtribology* broadly to both categorize a class of machines or moving assemblies that are small in scale (e.g., micromotors) as well as to describe tribological contacts that fall into the "space between" engineering scale devices and single asperities. Why is this important? Similar to large-scale systems, the design and implementation of small-scale sliding structures depends on understanding and predicting the durability of interfaces, but with the added complication that the interface may be composed of just a few contacting asperities. Do continuum models apply? What about surface effects or wear debris? The surface-to-volume ratio of small devices is also greater as size decreases, and surface forces (like capillary forces) that are not significant contributors in macroscale contacts may suddenly dominate. For this reason, geckos and flies can walk up walls and hang from ceilings using the many microscale hairs on their feet [1,2], while microdevices may realize only limited performance or exhibit complete seizure [3]. There are now many miniature devices in everyday products ranging from accelerometers controlling deployment of airbags in automobiles to inkjet heads in printers and mirror arrays in projectors [4,5]. The failures of these microelectromechanical systems (MEMS) or devices are dominated by adhesion, friction, and wear [5,6]. Thus, it is imperative to develop fundamental understanding of contacting interfaces comprising materials found in microscale systems with the appropriate scales. This is the regime of microtribology.

2.2 WHAT SCIENTIFIC ISSUES AND QUESTIONS SPAN THE GAP?

Perhaps the biggest challenge facing the experimental tribologist is how to devise and perform well-conceived experiments to simply compare friction and wear behavior at different scales. Multiple instruments will likely be used, and it will be necessary to make choices or compromises across the range of loads, contact stresses, sliding speeds, contact dimensions, geometry, and materials. Many of these topics are treated in detail in other chapters comprising this book. Take, for example, the simple experimental configuration of two counterbodies, one spherical and the other planar. This is referred to as sphere-on-flat geometry. This geometry is advantageous in the laboratory for two reasons. First, it minimizes sample alignment problems inherent in cylindrical or flat-on-flat geometries. Further, analytical expressions to evaluate elastic contact parameters (e.g., contact width, deformation, pressure, etc.), widely known as *Hertzian contact mechanics*, are used [7,8]. In the absence of adhesion, the projected contact size, a, is given by

$$a = \left(\frac{3PR}{4E_r} \right)^{1/3}$$

where P is the applied load, R is the radius of the sphere, and E_r is the reduced modulus

$$E_r = \left[\left(1 - \nu_1^2\right) / E_1 + \left(1 - \nu_2^2\right) / E_2 \right]^{-1}$$

with E_1, E_2, ν_1, ν_2 as elastic moduli and Poisson's ratios of the two contacting materials [7]. Ideally, one could change a single parameter at will—for example the contact width—and examine the tribological consequences. Practically, this is very difficult to achieve due to limitations in instrumentation available across scales.

Figure 2.1 shows plots of how changing radius, modulus, and load affect the average contact pressure, or load, divided by the projected contact area, where a is the

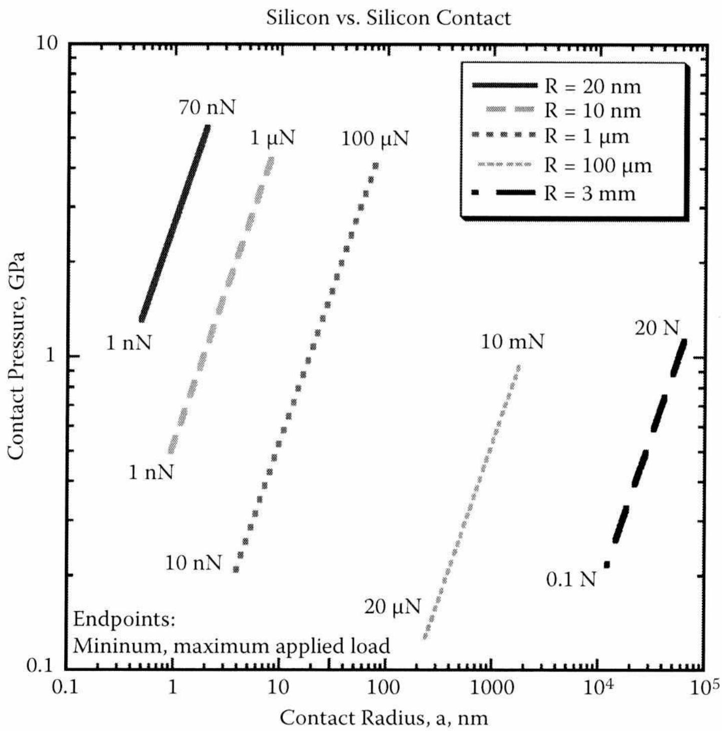

FIGURE 2.1 Hertz contact radius vs. average contact pressure calculated for silicon–silicon contacts for load and radius combinations representative of what can be achieved with a macroscopic pin-on-disk tribometer (broad dashed line at far right), an atomic force microscope (AFM) (solid and medium dashed lines at left of plot), and for a micro-scale tribometer (dotted lines, center). From this plot, it is readily seen that comparisons across lateral scales in contact radius over many orders of magnitude is possible.

radius of a contact of circular cross section ($P/\pi a^2$). This analysis assumes that roughness does not contribute and that the predicted contact area is equal to the true contact area. First, one can see that in comparing sliding experiments at different scales, it is a challenge to scale all parameters equally. For example, it would be very difficult to directly compare measurements made by AFM with a 20-nm radius tip to those made with a macroscopic tribometer under idealized conditions because the accessible load ranges and contact pressures are very different. However, with judicious selection of counterbody radius, a set of experiments might be performed to compare tribological response over a range of contact dimensions at similar stress ranges.

To illustrate further the challenges in scaling systems, we can look at how researchers developing MEMS structures [9] have attempted to compare and predict friction performance with a variety of test geometries and scales. For example, can friction behavior of a given macroscopic contact predict performance of microscale devices? What experimental materials and interface parameters are important (load, sliding speed, time between contacts, capillary forces, roughness, etc.)?

Figure 2.2 shows a summary of macroscopic and microscopic MEMS tribometer test configurations (upper) and data (lower) for a variety of materials combinations. The figure summarizes data from an assortment of macroscopic and microscopic experiments, where static friction coefficient (the force resisting initiation of sliding motion, relative to the applied load) is compared for various contact geometries, environments, and material combinations. While general trends for pin-on-disk or ball-on-disk geometries at higher loads reliably exhibit differences between air and vacuum environments (lower static friction in vacuum), values span nearly an order of magnitude. Macroscopic values are generally lower. Researchers could reliably perform experiments at lower loads and textured surfaces that may provide contacts more similar to those found in the MEMS devices (e.g., sidewall [11] and nanotractor [12,13] tribometers).

An additional point to notice regarding the simple pictures presented by Figures 2.1 and 2.2 is that it is not always possible to control or measure the experimental geometry confidently enough to definitively determine contact conditions such as average contact pressure. This is typically due to surface roughness or less-than-ideal counterface geometries. For example, researchers developing microscale actuators to make MEMS microtribometers from polycrystalline silicon (polysilicon) may be able to monitor the applied normal load and resulting static friction coefficient, but do not necessarily have a confident measure of kinetic friction (the force resisting sliding motion, relative to the applied load, during sliding), the contact area, or even how many asperities may be contributing to the contact phenomena. In this case, as demonstrated in Figure 2.2, researchers have been exploring comparisons between friction, or sometimes wear [13], measured by microdevices, and those measured using the same or similar materials using macroscopic tribometers.

Figure 2.3 diagrams the potential to perform experiments with overlap between macro-, micro-, and nanotribology regimes. The central rectangular region shows the approximate zone for experiments where the whole instrument and contact is microscale in dimension (e.g., MEMS device tribometer platforms) [10–14]. The right side, labeled "bulk," refers to typical pin-on-disk macrotribology experiments, and the left side is the regime typically accessible by AFM instrumentation.

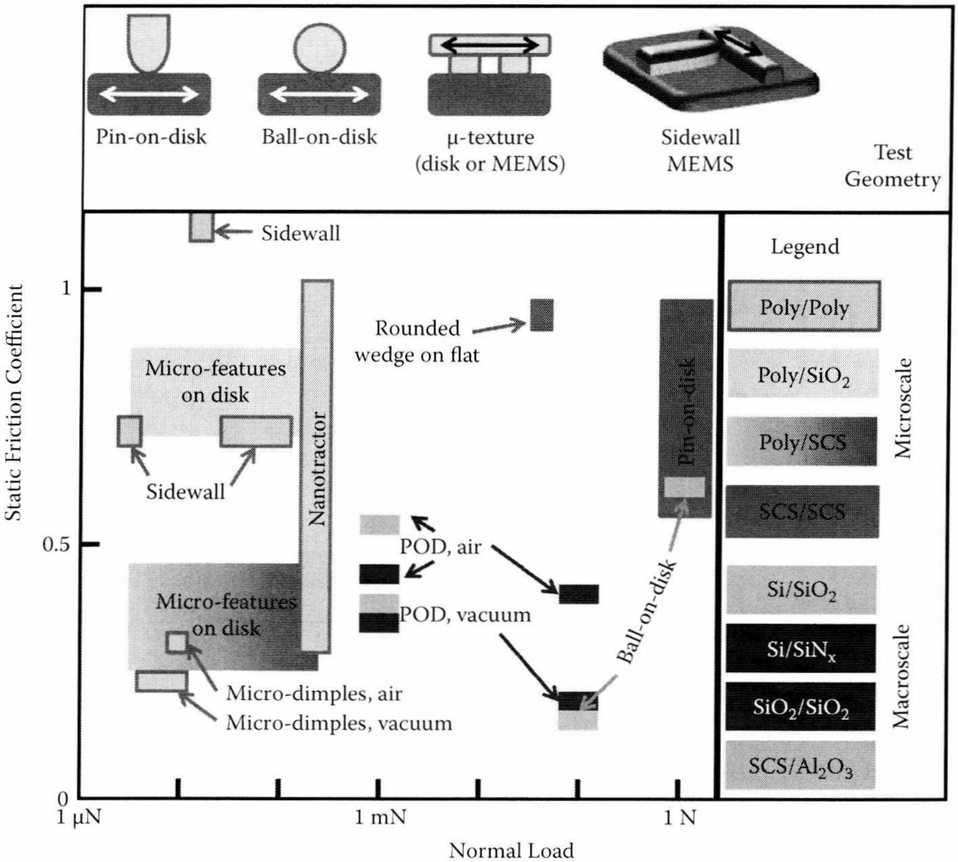

FIGURE 2.2 Comparison of microscale and macroscale static friction coefficient over a broad range of normal loads in air and vacuum environments. Materials in legend text include polysilicon (poly), silica (SiO2), single crystal silicon (SCS), substoichiometric silicon nitride (SiNx), and alumina (Al2O3). Adapted from Alsem, D.H., Dugger, M.T., Stach, E.A., and Ritchie, R.O. 2008. *J. Microelectromech. Sys.* 17, 1144–1154, Table 1, and including data from Lumbantobing, A., and Komvopoulos, K. 2005. *J. Microelectromech. Sys.* 14, 651–663.

In the middle are ovals depicting three regimes that have all been commonly referred to as "microtribology" in the scientific literature. The uppermost region is the regime accessible by commercial *scratch-testing* [15] instruments. In scratch-testing instruments, a sharp diamond tip is moved laterally across the sample (often a coated surface) while the load is increased linearly and the lateral force is monitored. The middle regime shows the approximate range of sliding nanoindentation experiments (with applied loads controlled between ~uN to ~mN) where the counterbody tips are much blunter than those used for scratch testing. On average, the blunter tip substantially reduces the contact stresses to GPa or lower. Contact stresses can be reduced further by employing larger counterface radii (e.g., 100 μm to mm scale) on a tribometer capable of controlling applying very low loads during sliding.