

## On the Scientific and Technological Importance of Nanotribology

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### ABSTRACT

Nanotribology has been in existence as a recognized discipline for roughly 20 years, with the appreciation of the importance of atomistic mechanisms of tribology existing long before. In this paper, we briefly review why nanotribology is important for advancing the science of tribology in general, and we also highlight emerging applications where nanotribological research is critical.

### INTRODUCTION

Nanotribology, the study of friction, adhesion, lubrication, and wear at the nanometer scale, is an interdisciplinary field where the fundamental origins of tribological phenomena are explored. While it is recognized as a basic science, it is also relevant to multiple commercial applications. Several detailed reviews of nanotribology already exist<sup>1-4</sup>, including a new monograph<sup>5</sup>.

### APPLICATION EXAMPLES

Computer hard disks are perhaps the most advanced and successful example of nanotribology applied to a commercial application<sup>5,6</sup>. In these systems, the magnetic media and the recording head are protected from mechanical and tribological contact with each other by diamond like carbon films only a few nanometers thick, and a lubricant coating only a few molecules thick. The fact that this system can operate for years with high fidelity in a range of environments demonstrates that tribological challenges can be successfully addressed at the nanoscale. In this example, the only dimension engineered at the nanoscale is normal to the surfaces.

In devices that are yet smaller in all dimensions, such as micro- and nano-electromechanical systems (MEMS/NEMS), surface forces and surface phenomena can dominate driving and inertial forces, and completely overwhelm gravity. This affects the fundamental design considerations for small devices and can seriously hinder functionality of a micro or nanodevice. As an example, silicon-based MEMS that involve contacting or sliding surfaces are often exhibit what is called "stiction", meaning parts stick together and cannot be separated (adhesion) or slid relative to one another (high static friction)<sup>7-9</sup>. Even when parts are able to slide, wear can be so high that the lifetime of the device is unsuitably low<sup>10,11</sup>. As of today, there are no commercially available MEMS devices that involve

surfaces in sliding contact. Devices with non-sliding (or perhaps with incipient sliding at most) do exist, such as the Digital Micromirror Device<sup>TM</sup> (DMD)<sup>12</sup>. The successful operation of this device required surface treatments to minimize adhesion, and fast mechanical pulses are applied continuously during operation to repeatedly break the contacting interfaces to prevent increases in adhesion with contact time.

In living systems, nanoscale interactions at interfaces control much of the function of the biological system as a whole. Examples where mechanical and tribological effects are critical include cell-surface interactions<sup>13</sup>, molecular motors<sup>14</sup>, and the packing of DNA into viruses<sup>15</sup>. For new and existing applications where synthetic devices interface with biological systems, such as drug delivery vehicles, diagnostics, engineered tissues, and orthopedic implants, the understanding of nano/bio interfaces is critical. Nanotribology has an increasingly important role to play in this complex, challenging arena.

### SCIENTIFIC APPROACHES

Traditionally, tribology has often focused on measuring friction coefficients and wear rates of materials for specific conditions. However, it has long been appreciated that both the friction coefficient and wear rate are not intrinsic physical properties. Both of these are often strongly dependent on the specific environmental conditions (temperature, gas atmosphere), the sliding velocity, the load, the roughness and cleanliness of the surfaces, and the sliding history of both surfaces. Measurements can also be affected by the mechanical stiffness and dynamics of the tribometer used to perform the measurements. If fundamental, predictive understanding is to be gained, then the complex nature of tribological systems requires that experiments be at extremely well-defined interfaces under well-defined conditions.

One approach that is enabled by nanotribology is to perform experiments at the level of single asperity contacts. Both measurements and simulations using single asperity contacts have already provided a range of insights. The primary tool used for experiments is atomic force microscopy (AFM)<sup>16,17</sup>. Over twenty years of technique developments in AFM have enabled force measurements in the sub-nanoNewton regime, and produced tribological measurements with

nanometer-scale spatial resolution on surfaces, where the contacts are of nanometer-scale dimensions. Atomistic simulations based on the molecular dynamics (MD) technique have been used to model single-asperity contacts as well as their dynamics during sliding. As mentioned above, many of these advances are reviewed in detail elsewhere<sup>1-5</sup>. There are several major challenges that confront nanotribologists, but two key ones of a technical nature emerge as perhaps the most pressing. First, the AFM technique still suffers from substantial uncertainty, specifically in the proper calibration of measured forces, and in knowing the precise composition and structure of the tip. Calibration techniques exist but are not uniformly applied<sup>18-26</sup>. Methods to characterize the tip are not as established and in fact there is no way to know the identity, position, and bonding state of every atom at the tip or sample in a nanoscale interface, but progress is being made such as through the use of *in-situ* techniques<sup>27-30</sup>. Further effort along these lines is needed.

The second challenge pertains to the simulations. The time scales are too rapid and the number of atoms too small, both by orders of magnitude, to enable exact comparisons with the conditions of experiments. In other words, the simulations are not for the same asperity size or the same sliding velocity as most experiments. Related to this, MD simulations are often carried out simply under vacuum environments, unlike most experiments. The size issue is becoming less of an issue as computation power increases and some MD studies now do match the size of experiments<sup>31</sup>, but velocities are still not matched. Efforts to take advantage of massive parallelization, accelerated MD techniques<sup>32</sup>, or other novel and creative developments are needed. The potentials used in MD simulations have been developed over many years with tremendous effort, but validation of these potentials by rigorous, testable means is lacking. A more careful examination of the effects of the assumptions and approximations of classical, empirical MD potentials when simulating tribological interfaces should be carried out.

Using nanotribology to explain and predict tribology phenomena in a general way is perhaps a “grand challenge” for the field of tribology as a whole. Close collaboration and communication between nanotribologists and macrotribologists is critical. It is also critical that nanotribologists, regardless of their background, familiarize themselves with the extensive literature of contact mechanics and tribology. While much of the published work may have a specific and engineering-based focus, there is a tremendous amount of knowledge and a remarkable range of phenomena explored and explained by tribologists that merits appreciation by the newer community of nanotribologists. This work can help nanotribologists to properly choose materials, conditions, and scientific questions which are truly relevant to solving important problems in tribology.

The suggestions above are merely a few of many that are worthy of consideration. The key conclusion is that major opportunities exist for nanotribology to have a significant

impact on both our scientific understanding of tribology in general, and on a range of technologically and commercially important applications. Whether or not this succeeds will depend on how forward-thinking, open, and communicative the community is, and the extent to which it pursues rigor and excellence using the highest standards of science and engineering.

## REFERENCES

1. I. Szlufarska, M. Chandross & R. W. Carpick, "Recent Advances in Single-Asperity Nanotribology". *J. Phys. D: Appl. Phys.* **41**, 123001/1 (2008)
2. E. Gnecco, R. Bennewitz, T. Gyalog & E. Meyer, "Friction experiments on the nanometre scale". *J. Phys., Condens. Matter.* **13**, R619 (2001)
3. R. W. Carpick & M. Salmeron, "Scratching the surface: Fundamental investigations of tribology with atomic force microscopy". *Chem. Rev.* **97**, 1163 (1997)
4. I. L. Singer & H. M. Pollock (eds.) *Fundamentals of Friction: Macroscopic and Microscopic Processes* (Kluwer, Dordrecht, 1992).
5. C. M. Mate, *Tribology on the small scale : a bottom up approach to friction, lubrication, and wear* (Oxford University Press, Oxford ; New York, 2008).
6. B. Marchon, "Head/disk tribology: toward 10 Gb/in<sup>2</sup>". *J. Appl. Phys.* **79**, 4508 (1996)
7. R. Maboudian, W. R. Ashurst & C. Carraro, "Tribological challenges in micromechanical systems". *Trib. Lett.* **12**, 95 (2002)
8. R. Maboudian & R. T. Howe, "Critical review: Adhesion in surface micromechanical structures". *J. Vac. Sci. Technol.* **15**, 1 (1997)
9. M. P. de Boer & T. M. Mayer, "Tribology of MEMS". *MRS Bulletin* **26**, 302 (2001)
10. E. E. Flater, A. D. Corwin, M. P. de Boer & R. W. Carpick, "In-situ wear studies of surface micromachined interfaces subject to controlled loading". *Wear* **260**, 580 (2006)
11. A. D. Romig, Jr., M. T. Dugger & P. J. McWhorter, "Materials issues in microelectromechanical devices: science, engineering, manufacturability and reliability". *Acta Mat.* **51**, 5837 (2003) [http://dx.doi.org/10.1016/S1359-6454\(03\)00440-3](http://dx.doi.org/10.1016/S1359-6454(03)00440-3)
12. S. A. Henck, "Lubrication of Digital Micromirror Devices<sup>TM</sup>". *Trib. Lett.* **3**, 239 (1997) <http://dx.doi.org/10.1023/A:1019129021492>
13. D. E. Discher, P. Janmey & Y. L. Wang, "Tissue cells feel and respond to the stiffness of their substrate. " *Science* **310**, 1139 (2005)
14. Y. Ahimet, J. N. Forkey, S. A. McKinney, T. Ha, Y. E. Goldman & P. R. Selvin, "Myosin V walks hand-over-hand: single fluorophore imaging with 1.5-nm localization". *Science* **300**, 2061 (2003) <http://dx.doi.org/10.1126/science.1084398>

15. P. K. Purohit, M. M. Inamdar, P. D. Grayson, T. M. Squires, J. Kondev & R. Phillips, "Forces during bacteriophage DNA packaging and ejection". *Biophysical Journal* **88**, 851 (2005)  
<http://dx.doi.org/10.1529/biophysj.104.047134>
16. A. W. Homola, J. N. Israelachvili, P. M. McGuiggan & M. L. Gee, "Fundamental experimental studies in tribology: The transition from interfacial friction of undamaged molecularly smooth surfaces to normal friction and wear". *Wear* **136**, 65 (1990)
17. A. D. Berman, W. A. Ducker & J. N. Israelachvili, "Origin and Characterization of Different Stick-Slip Friction Mechanisms". *Langmuir* **12**, 4559 (1996)
18. M. Tortonese & M. Kirk, "Characterization of application specific probes for SPMs". *Proc. SPIE - Int. Soc. Opt. Eng.* **3009**, 53 (1997)
19. R. J. Cannara, M. Eglin & R. W. Carpick, "Lateral force calibration in atomic force microscopy: A new lateral force calibration method and general guidelines for optimization". *Rev. Sci. Instrum.* **77**, 53701/1 (2006)  
<http://dx.doi.org/10.1063/1.2198768>
20. J. Stiernstedt, M. W. Rutland & P. Attard, "A novel technique for the in situ calibration and measurement of friction with the atomic force microscope". *Rev. Sci. Instrum.* **76**, 83710 (2005)  
<http://dx.doi.org/10.1063/1.2006407>
21. C. P. Green, H. Lioe, J. P. Cleveland, R. Proksch, P. Mulvaney & J. E. Sader, "Normal and torsional spring constants of atomic force microscope cantilevers". *Rev. Sci. Instrum.* **75**, 1988 (2004)  
<http://dx.doi.org/10.1063/1.1753100>
22. M. Varenberg, I. Etsion & G. Halperin, "An improved wedge calibration method for lateral force in atomic force microscopy". *Rev. Sci. Instrum.* **74**, 3362 (2003)
23. J. E. Sader, J. W. M. Chon & P. Mulvaney, "Calibration of rectangular atomic force microscope cantilevers". *Rev. Sci. Instrum.* **70**, 3967 (1999)
24. D. F. Ogletree, R. W. Carpick & M. Salmeron, "Calibration of frictional forces in atomic force microscopy". *Rev. Sci. Instrum.* **67**, 3298 (1996)
25. J. E. Sader & C. P. Green, "In-plane deformation of cantilever plates with applications to lateral force microscopy". *Rev. Sci. Instrum.* **75**, 878 (2004)  
<http://dx.doi.org/10.1063/1.1667252>
26. V. S. J. Craig & C. Neto, "In situ calibration of colloid probe cantilevers in force microscopy: hydrodynamic drag on a sphere approaching a wall". *Langmuir* **17**, 6018 (2001)
27. C. A. Schuh, "Nanoindentation studies of materials". *Materials Today* **9**, 32 (2006)
28. O. L. Warren, Z. W. Shan, S. A. S. Asif, E. A. Stach, J. W. Morris & A. M. Minor, "In situ nanoindentation in TEM". *Materials Today* **10**, 59 (2007)
29. R. Ribeiro, Z. Shan, A. M. Minor & H. Liang, "In situ observation of nano-abrasive wear". *Wear* **263**, 1556 (2007)
30. A. P. Merkle & L. D. Marks, "Friction in full view". *Appl. Phys. Lett.* **90**, 064101 (2007)
31. M. Chandross, C. D. Lorenz, M. Stevens & G. S. Grest, "Simulations of nanotribology with realistic probe tip models". *Langmuir* **24**, 1240 (2008)
32. A. F. Voter, F. Montalenti & T. C. Germann, "Extending the time scale in atomistic simulation of materials". *Annu. Rev. Mater. Res.* **32**, 321 (2002)