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Education

Ph.D. Mechanics and Tribology, Tsinghua University, 1999
M.S. Solid Mechanics, Tsinghua University, 1987
B.S. Mechanical Engineering, North China University of Technology, 1984

Teaching

MAE 167 Mechanics of Materials Lab. (Fall)
ApSc 130 Materials Science (Spring)

Research

Dr. Leng's research group currently focuses on several fundamental issues related to computational materials science at nanometer scales, particularly in the area of surface and interfacial science. Research interests include computational nanotribology — the science of adhesion, friction and lubrication at nanometer scales, molecular modeling of self-assembly at organo-metallic interfaces, mechanical property of metal nanowires and the development of computational methodology.

1. Hydration Force, Hydrophobic Interaction, and Shear Dynamics in Nanometer Confined Aqueous Films

The mechanical properties of aqueous films under nanometer confinement have many implications in materials science and engineering at nanometer scales. Adhesion and wetting, friction and lubrication in micro/nano electro-mechanical systems (M/NEMS) are among typical examples. Many biological processes, such as interactions between biomembranes, water transport through ion channels and through crowded intracellular environment, protein folding, and biolubrication also involve water and ions under extreme confinements. This research is closely related to the surface force balance (SFB)

experiments by Jacob Klein's group at Weizmann Institute of Science and Oxford University. With the support of NSF and DoD funding, current research interests include hydration structure and repulsive hydration force mechanism between two charged surfaces in aqueous environment, water depletion and hydrophobic collapse between hydrophobic surfaces in water, internal dynamics of water molecules and hydrated ions, shear response of hydration layers, and boundary slip at liquid/solid interfaces. Thermodynamic properties of non-aqueous liquids under nanometer confinement are also under investigation in this group.

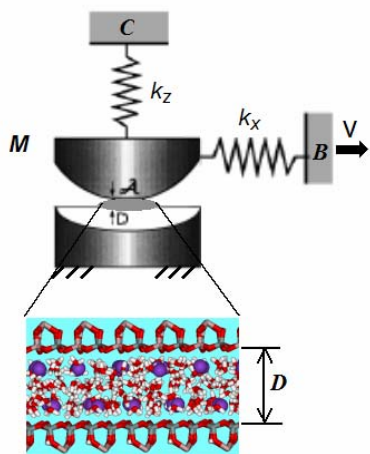


Figure 1. A mechanical molecular model in surface force balance (SFB) experiment.

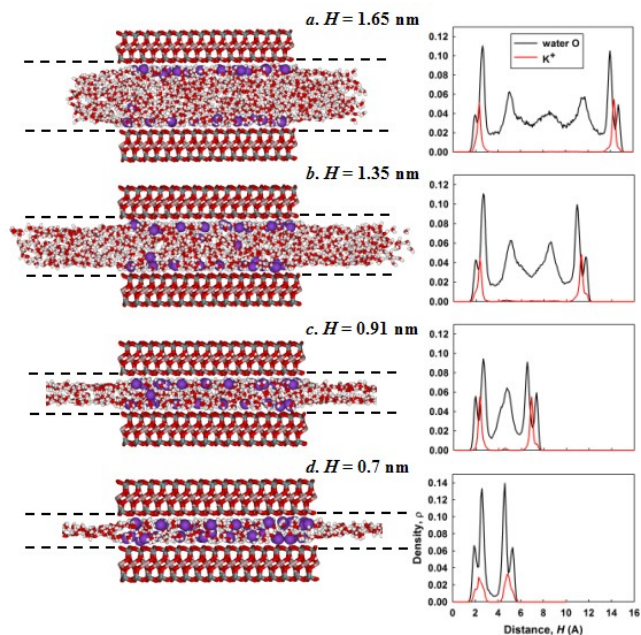


Figure 2. Water and ions hydration structure and density distributions between two charged mica surfaces.

Selected publications

1. Leng, Y. S. Hydration force and dynamic squeeze-out of hydration water under subnanometer confinement. *Journal of Physics: Condensed Matter* **20**, 354017 (2008).
2. Xu, D. Y., Li, D. Y., Leng, Y. S. and Chen, Y. F. Molecular dynamics simulations of ion distribution in nanochannels. *Molecular Simulation* **33**, 965 (2007).
3. Leng, Y. S. and Cummings, P. T. Shear dynamics of hydration layers. *Journal of Chemical Physics* **125**, 104701 (2006).
4. Leng, Y. S. and Cummings, P. T. Structure of hydration water confined between mica surfaces. *Journal of Chemical Physics* **124**, 74711 (2006).
5. Leng, Y. S. and Cummings, P. T. Fluidity of hydration layers nanoconfined between mica surfaces. *Physical Review Letters*, **94**, 026101 (2005).

2. Bonding and Packing Structure at Organo-metallic Interfaces. Mechanical Property of Metal Nanowires

The purpose of this research is to understand the chemical bonding and packing structure of organic self-assembled monolayers (SAMs) on metal surfaces and clusters. This research has many practical applications in nanotechnology, such as catalysis, structural materials, electronic materials, and molecular electronic devices. Current research interests include the classical force field development from quantum mechanical calculations for the organo-metallic complexes and molecular simulations of self-assembly. Mechanical elongation behavior of gold nanowires is a closely related topic in this research. Using the tight-binding second momentum potential for transition metals, we demonstrate that there exists a universal law — the rate-dependent energy release mechanism to control the formation of different metal junction structures.

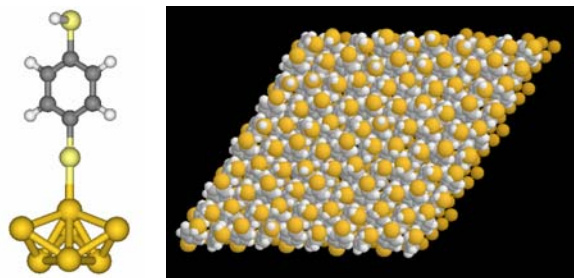


Figure 3. Benzenedithiolate (BDT) molecule bonded with 7-gold cluster and the packing structure of BDT monolayer on Au (111) surface.

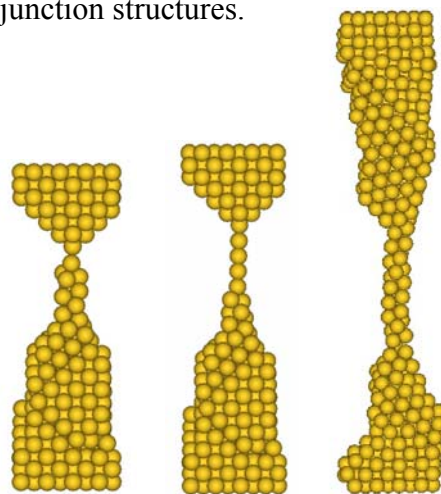


Figure 4. Depending on elongation rate, temperature and system size, the elongated gold junction structure before break can be a shorter or longer monatomic chain, or a completely different helical structure.

Selected publications

1. Pu, Q., Leng, Y. S., Cummings, P. T. The rate-dependent energy release mechanism of gold nanowires under elongation (*Submitted to Journal of the American Chemical Society*).
2. Pu, Q., Leng, Y. S., Zhao, X. C., and Cummings, P. T. Molecular simulations of stretching gold nanowires in solvents. *Nanotechnology* **18**, 424007 (2007).
3. Leng, Y. S., Dyer, P. J., Krstić, P. S., Harrison, R. J., and Cummings, P. T. Calibration of chemical bonding between benzenedithiolate and gold: the effects of geometry and size of gold clusters. *Molecular Physics* **105**, 293 (2007).
4. Pu, Q., Leng, Y. S., Tsetseris, L., Park, H. S., Pantelides, S. T., and Cummings, P. T. Molecular dynamics simulations of stretched gold nanowires — the relative utility of different semiempirical potentials. *Journal of Chemical Physics* **126**, 144707 (2007).

5. Leng, Y. S., Krstić, P. S., Wells, J. C., Cummings, P. T., and Dean, D. J. Interaction between benzenedithiolate and gold: Classical force field for chemical bonding. *Journal of Chemical Physics*, **122**, 244721 (2005).
6. Leng, Y. S., Keffer, D. J. and Cummings, P. T. Structure and dynamics of a benzenedithiol monolayer on a Au (111) surface. *Journal of Physical Chemistry B*, **107**, 11940 (2003).

3. Nano-contact mechanics in atomic force microscope (AFM)

Continuum contact mechanics and molecular simulation approaches are combined to explore the mechanisms of adhesion and friction, energy dissipation in atomic force microscope (AFM) and chemical force microscope (CFM) experiments. Understanding these fundamental issues is critical to control the nanoscale imaging process in AFM and friction in M/NEMS. Details include investigations of contact pressure distributions, nanoscale deformation, adhesion hysteresis, stick-slip and binding forces between biomolecules. Development of multiscale hybrid molecular simulation method to overcome the time- and length-scale difficulties in molecular level simulations is an important topic in this research.

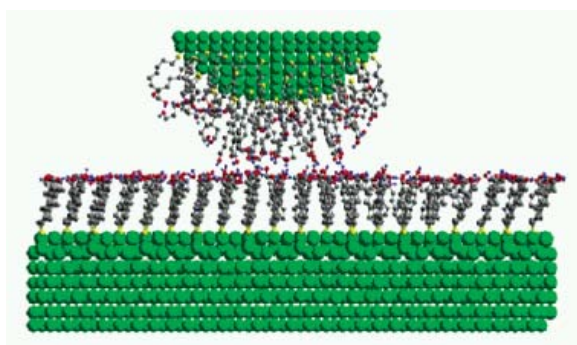


Figure 5. Binding between a model AFM tip passivated by alkanethiolate (AT) molecules with AT monolayer on a gold (111) surface.

Selected publications

1. Zhou, J., Zhang, L. Z., Leng, Y. S., Tsao, H. K., Sheng, Y. J., Jiang, S. Y. Unbinding of the streptavidin-biotin complex by atomic force microscopy: A hybrid simulation study. *Journal of Chemical Physics* **125**, 104905 (2006).
2. Leng, Y. S. and Jiang, S. Y. Dynamic simulations of adhesion and friction in chemical force microscopy. *Journal of the American Chemical Society*, **124**, 11764 (2002).
3. Leng, Y. S. and Jiang, S. Y. Slow dynamics in atomic force microscopy. *Physical Review B*, **63**, 193406 (2001).
4. Leng, Y. S. and Jiang, S. Y. Dissipative process in atomic force microscopy. *Physical Review B*, **64**, 115415 (2001).
5. Leng, Y. S. and Jiang, S. Y. Atomic indentation and friction of self-assembled monolayers by hybrid molecular simulations. *Journal of Chemical Physics*, **113**, 8800 (2000).
6. Leng, Y. S., Hu, Y. Z., and Zheng, L. Q. Adhesion of smoothly flat-ended wedges. *Proc. R. Soc. Lond. A*, **456**, 185 (2000).