Monday 4th, Morning

8h50-9h20 Registration

9h20-9h30 Opening remarks

9h30-9h40 Introduction by WG1 leader

Session chair: Michael Urbakh

9h40-10h20: Eran Bouchbinder
Dynamic stability of frictional sliding

10h20-10h40 Mona Mahboob Kanafi
Effect of macro/micro-roughness on rubber friction: Combining field and laboratory experiments

10h00-11h40 Coffee break

11h40-12h00 Andra Craciun
Stochastic nanoscale stick-slip friction on oxides

12h00-12h40 Bo Persson
Soft matter dynamics: accelerated fluid squeeze-out during slip

12h40-13h00 Lunch break

DYNAMIC STABILITY OF FRICTIONAL SLIDING

Eran Bouchbinder

Weizmann Institute of Science, Department of Chemical Physics, 7610001 Rehovot, Israel

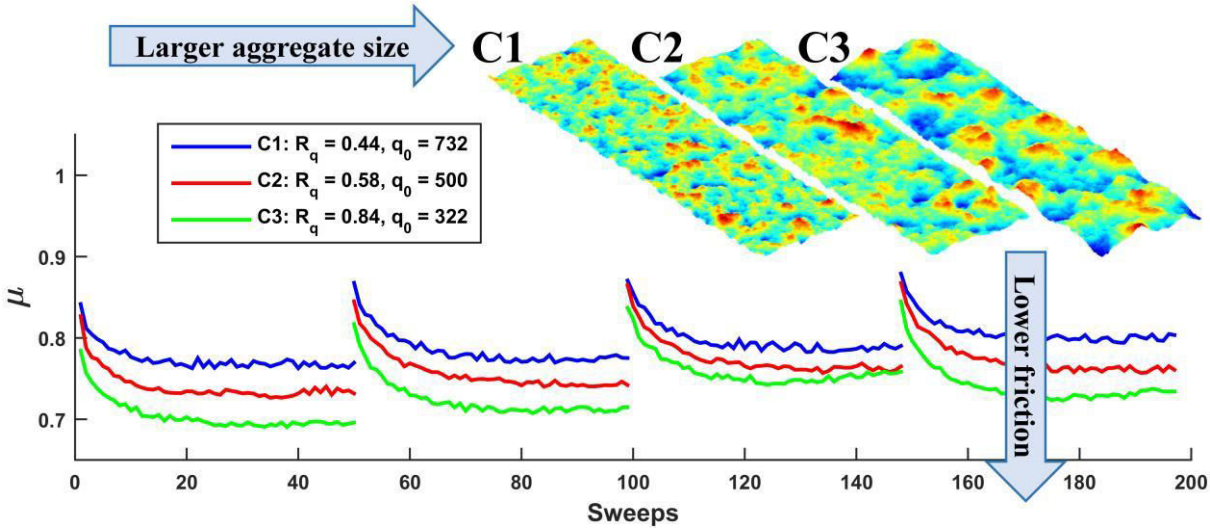
In this talk I will review our recent progress in understanding the dynamic stability of frictional sliding along spatially-extended interfaces. Spatial attention will be given to the interplay between the interfacial constitutive law, in particular, instantaneous and steady-state velocity-strengthening response and generic properties of the sliding bulks, in particular, material contrast across the interface, the finite geometry and the loading configuration. The emerging instabilities and a stability phase-diagram will be discussed, along with various applications.

EFFECT OF MACRO/MICRO-ROUGHNESS ON RUBBER FRICTION: COMBINING FIELD AND LABORATORY EXPERIMENTS

Mona Mahboob Kanafi and Ari Tuononen

Vehicle Engineering Group, School of Engineering, Aalto University, P.O. Box 14300, FI-00076 Aalto, Helsinki, Finland

The significant impact of surface roughness characteristics on determining the friction of bodies in tribo-systems is well recognized. The link between road pavement macro/micro-roughness and friction calls for surface roughness indicators that could best describe the multiscale nature of the road top topography, where the actual contact occurs. In this manner, a thorough field experiment was conducted on existing road pavements to elucidate qualitative link between scale independent roughness parameters and road pavement friction at actual road conditions. But the exploration of the exact connection between macro/micro-scale roughness and friction is not feasible at field conditions. Hence, experimental work was extended to a set of laboratory examinations to enforce control over texture parameters. Here, 3D printing technology was utilized to generate artificial geometries with carefully selected surface characteristics on the basis of the random process theory and fractal modelling. Sliding friction experiments on the printed surfaces demonstrated that this novel method can improve our understanding of the texture impacts on friction.



Friction versus number of sweeps for 3D printed artificial surfaces with different root-mean-square roughness (R_q) and roll-off wavevector (q_0) combinations.

STOCHASTIC NANOSCALE STICK-SLIP FRICTION ON OXIDES

A. D. Craciun, J. L. Gallani and M. V. Rastei

Institut de Physique et Chimie des Matériaux de Strasbourg, CNRS, Université de Strasbourg, F-67034

Friction mechanism has been widely investigated on atomic level, most of the models being based on a Prandtl-Tomlinson approach [1, 2]. Nevertheless, friction on amorphous surfaces is scarcely reported, despite the fact that for example, in the case of micro- and nano-mechanical devices we are dealing with sliding surfaces covered by native oxides [3,4]. Here, we report a nanoscale stick-slip friction mechanism present at the interface between an AFM tip and various oxide surfaces. Experiments reveal a stochastic stick-slip behavior with stick phases extending to several nanometers (see Figure 1). A linear scaling of friction force with normal load along with low pull-off forces indicates dispersive adhesive interactions at the interface. The influence of thermal effects on the stick-slip process is equally investigated. Our findings are explained by a variable Lennard-Jones-like interaction potential model [5,6]. The model explains the formation and fluctuation of the erratic stick-slip events and provides information regarding the impact of external parameters on nanoscale friction on oxide surfaces.

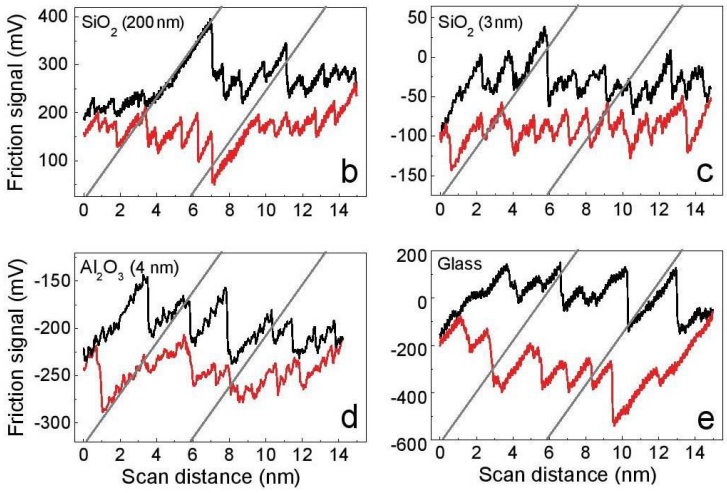


Figure 1. Friction loops for different oxide surfaces

[1] Gnecco E., Bennewitz R., Gyalog T., Loppacher Ch.,Bammerlin M., Meyer E. and Güntherodt H-J, Phys. Rev. Lett. 84 1172 (2000)

[2] Krylov S. Yu, Jinesh K. B., Valk H., Dienwiebel M. and Frenken J. W. M., Phys. Rev. E 71 065101 (2005)

[3] Schirmeisen A., Jansen L., Holscher H.,Fuchs H., Appl. Phys. Lett 88, 123108 (2006)

[4] Lessel M., Loskill P., Hausen F., Gosvami N., Bennewitz R., Jacobs K.,Phys. Rev. Lett. 111, 35502 (2013)

[5] Craciun A. D., Beyer N, Gallani J.L., Rastei M. V., Nanotechnology 27, 055402 (2016)

[6] Pinon A. V., Wierez-Kien M., Craciun A. D., Beyer N, Gallani J.L., Rastei M. V., Phys. Rev. B 93, 035424 (2016)

SOFT MATTER DYNAMICS: ACCELERATED FLUID SQUEEZE-OUT DURING SLIP

B.N.J. Persson

PGI-1, FZ Jülich, Germany, EU, and www.MultiscaleConsulting.com

Using a Leonardo da Vinci experimental set-up (constant driving force), I study the dependency of lubricated rubber friction on the time of stationary contact and on the sliding distance. I slide rectangular rubber blocks on smooth polymer surfaces lubricated by glycerol or by a grease. I observe a remarkable effect: during stationary contact the lubricant is only very slowly removed from the rubber-polymer interface, while during slip it is very rapidly removed resulting in a slip distance typically of order only a few times the length of the rubber block in the sliding direction. For an elastically stiff material, Poly(methyl methacrylate) (PMMA) I observe the opposite effect: the sliding speed increases with time (acceleration), and the lubricant film thickness appear to increase. I propose a novel explanation for the observed effect based on transient elastohydrodynamics, which may be relevant also for other soft contacts. I also present calculated Stribeck curves (friction as a function of the sliding speed) for surfaces with unisotropic roughness, and compare to measured results.

Monday 4th, Afternoon

Session chair: Zhenyu J. Zhang

13h40-14h20 Nuria Espallargas
Effect of surface oxides on friction and wear of metals and ceramic-metallic materials

14h20-14h40 Kostyantyn Grinkevych
Aircraft lubricant materials with functional additives of graphene-like molybdenum diselenide nanoparticles as new solid 2D nanolubricants

14h40-15h00 Alex Laikhtman
The effect of rhenium doped fullerene-like molybdenum disulfide nanoparticles on friction and wear

15h00-16h00 Coffee break

16h00-16h20 Florence Vivier
Interaction study between components in friction pad material

16h20-16h40 Peter Reininger
Experimental characterization and modeling of friction at the head/tape interface

EFFECT OF SURFACE OXIDES ON FRICTION AND WEAR OF METALS AND CERAMIC-METALLIC MATERIALS

Nuria Espallargas

Tribology Lab, Department of Engineering Design and Materials, Faculty of Engineering and Technology, Norwegian University of Science and Technology (NTNU), Trondheim, Norway, E-mail: nuria.espallargas@ntnu.no

Surface metal oxides are the result of the reaction of oxygen with metals in air or in water. Metal oxides on surfaces can be formed by the spontaneous reaction of metals with oxygen in the presence of a liquid electrolyte to protect against corrosion (i.e. passivation) or they can be the result of a tribological process (i.e. tribofilm). These chemical species formed on the surface play a very important role when solid materials such as metals or metal-ceramics are subjected to motion in contact with other bodies (i.e. tribological contacts). Understanding the role of surface oxides on friction and wear has been a widely studied topic in tribology, especially at the macroscale and from an engineering perspective [1-3]. These studies have led to proposing different mechanisms for friction and wear from an empirical perspective, although lately the more fundamental aspects of friction are emerging and atomic-scale studies are becoming more and more relevant [4].

There are several engineering applications where oxides are unavoidably present or generated on the surface of materials in relative motion. These surface oxides can be beneficial in some applications leading to decrease friction due to a self-lubricating effect, but in some circumstances they can lead to increase friction even if the same pair of materials is interacting. In addition, surface oxides may lead to considerably increase wear, being tribocorrosion a clear example of it [5].

In this work the effect of surface metal oxides on friction and wear of metal and ceramic-metallic pairs will be presented. The effect of environment, humidity, electrode potential, type of contact and microstructure on wear and friction will be discussed and analyzed from the macro- to the nano-scale.

[1] A.R.C Westwood and F.E. Lockwood. Tribology series 7. Elsevier (1981).

[2] Solid Lubrication and Surface Treatments, In: Tribology Series, Elsevier, 1993, Volume 24, pp 485-526.

[3] J.A.R. Wesmann and N. Espallargas. Tribology International 94 (2016) 360- 372.

[4] Michael Urbakh and Ernst Meyer, Nature materials 9 (2010) 8-10.

[5] A. Igual Muñoz and N. Espallargas, Tribocorrosion mechanisms in sliding contacts, In Woodhead Publishing Series in Metals and Surface Engineering, 2011, pp 118-152.

AIRCRAFT LUBRICANT MATERIALS WITH FUNCTIONAL ADDITIVES OF GRAPHENE-LIKE MOLYDENUM DISELENIDE NANOPARTICLES AS NEW SOLID 2D NANOLUBRICANTS

K. Grinkevych, L. Kulikov and N. Konig-Ettel

Institute for Problems of Materials Science, National Academy of Science of Ukraine, Kyiv, Ukraine

The development of the multifunction oils effective for most of friction units with the advent of new, modern aircraft becomes complicated. It is expected that high-temperature oils with additives of a new generation of 2D solid nanolubricants as graphene-like Molybdenum Diselenide (2H-$MoSe_2$) nanoparticles will have number of advantages in tribological characteristics at extreme operating conditions compared to well-known analogues of leading world manufacturers.

Systematic investigations of tribological characteristics of high-temperature aircraft oils (BP Turbo, Oil 2380, MS-8p and IPM-10; industrial I-20A oil as a basis for comparison) with functional additives of 2H-$MoSe_2$ as solid 2D nanolubricants are carried out for the first time. Homogenous graphene-like nanoparticles 2H-$MoSe_2$ (average sizes at [013] and [110] directions: d[013]=5,5(3) nm, d[110]=26,8(1,7) nm) was proposed as multifunctional 2D additives.

For the first time the effectiveness of these additives to universal aircraft oils was studied in a wide range of speed-load modes, including dynamic loading. The experiments at the original tribocomplex CATC were carried out. The CATC is tribocomplex of module type that consists of multipurpose tribotest machine, friction unit with the dynamic loading, computer and complex of electronic devices which provide the multiparameter control and information processing in real-time. The CATC allowed to conduct tests of three types: (i) all modes of lubricating action from boundary to hydrodynamical at “plane – generatrix of cone” scheme depending on loading and speed regimes, (ii) quasi-static wear test with reciprocation sliding indenter by the “plane – sphere” scheme performed at quasi-static load (30 N) applied in a normal direction to the tested surface and (iii) so-called dynamic wear test, which consist in applying both the quasi-static and alternating components of load. Amplitude of load alternating component was approx 10 % of quasi-static one. Friction force, wear, electrical contact resistance, triboelectromotive force of samples were studied in situ.

The proposed test schemes allowed to evaluate the influence of oil and additive on tribological (including tribophysical) characteristics of lubricant materials for studied lubricating modes. The addition of graphene-like 2H-$MoSe_2$ nanoparticles reduced wear for all studied lubricant compositions in 1.25–6 times in comparison with the base oils depending on the load-speed test conditions. The influence of rotation frequency on the tribosystem parameters have shown that the lubricant compositions, especially based on BP Turbo Oil 2380, had a higher lubricity (the smallest wear and speed up to the establishment of the hydrodynamic regime). Less viscosity of MS-8p oil and its compositions provided less lubricity, as evidenced decrease by an order of the electrical parameters in comparison with more viscous other oils. However, the additive of graphene-like 2H-$MoSe_2$ to MS-8p oil was more effective at boundary lubrication conditions.

In general, in these tribosystems wear protection determined by probable interaction of 2D inorganic nanoparticles (2H-$MoSe_2$) with organic components of oils at specific conditions of tribochemical processes and possible formation of 2D nanocomposites (“nanotribosynthesis”), and closely linked to tribophysical properties of 2D nanoparticles, lubricating capacity and physical-chemical properties of base oils.

The obtained test results of oils with additives of graphene-like Molybdenum Diselenide nanoparticles indicate the prospects of their use for design of 2D nanolubricant materials of new generation.

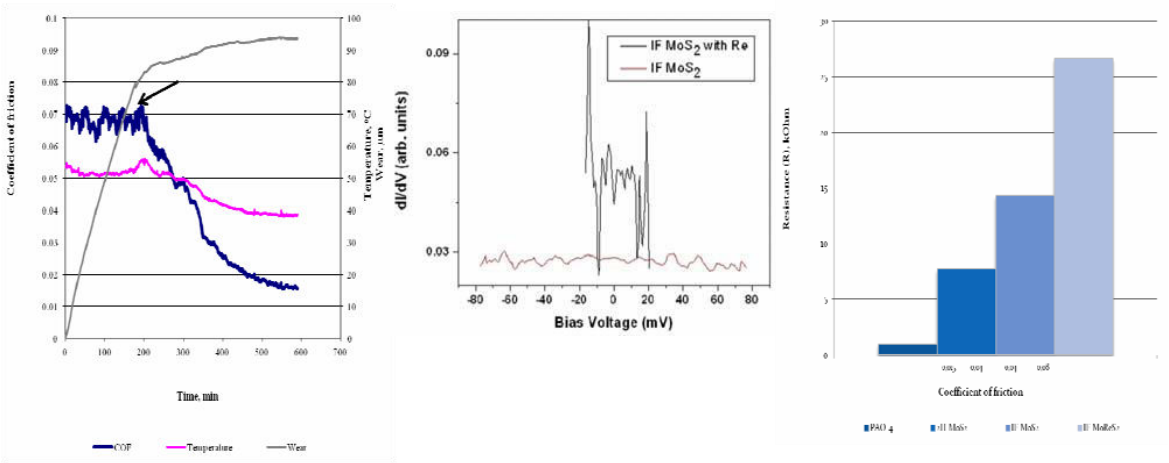
THE EFFECT OF RHENIUM DOPED FULLERENE-LIKE MOLYBDENUM DISULFIDE NANOPARTICLES ON FRICTION AND WEAR

Alex Laikhtman[1], Lev Rapoport[1], Alexey Moshkovich[1], Vladislav Perfilyev[1] and Reshef Tenne[2]

[1] Holon Institute of Technology (HIT), Holon, 5810201, Israel
[2] Weizmann Institute of Science, Rehovot, 7610001, Israel

Inorganic fullerene-like (IF) nanoparticles (NP) of WS_2 and MoS_2 exhibit very good tribological behavior as additives to lubricating fluids and as self-lubricating coatings and for improving the mechanical behavior of nanocomposites. Since the IF NP of WS_2 and MoS_2 are semiconducting materials, the conduction electrons near the NP surface are expected to affect many of their properties including their friction and wear behavior. It is believed that the excess electrons produced by the substitutional rhenium doping are trapped by defects on the NP surface. The negatively charged colloidal NP, which are surrounded by a positively charged ionic atmosphere, repel each other at close proximity and are therefore much less agglomerated than their undoped counterparts. The doped NP were characterized by different methods. In particular, the Re atoms at concentrations < 0.1 at% were found to substitute the Mo lattice atoms and donate electron to the conduction band making the NP negatively charged. Application of Re-IF-MoS_2 NP provides an ultra-low friction coefficient and a very low wear rate. The unique tribological properties of Re-doped NP can be related to the rolling effect of the NP and tribocharging of the tribofilms by the surface layer of Re:IF-MoS_2 NP. Based on the STS analysis it is suggested that the Re doped NP are more conductive then undoped MoS_2 NP. SEM, AFM and a measurement of the electrical resistance demonstrate formation of a smooth and dense Re-IF-MoS_2 solid lubricant film on the rubbed surfaces.

(1) **(2)** **(3)**



(1) The dependences of the friction coefficient (COF), temperature and wear vs. time;
(2) STS spectra from IF-MoS_2 and Re-doped (0.12 at%) IF-MoS_2 NP;
(3) Electrical resistance of the disks rubbed with pure oil and oil with 2H-MoS_2, IF-MoS_2 and Re-IF-MoS_2 NP.

INTERACTION STUDY BETWEEN COMPONENTS IN FRICTION PAD MATERIAL

Florence Vivier and Diego Pellerej

ITT Italia Srl

Brake pad formulations usually contain more than 15 components. Even if the effect of each filler on the final product properties are known (mainly friction coefficient and wear rate), the precise contribution of each ingredient remain unclear. The study of each singular filler contribution is very difficult considering the complexity of all the interaction co-existing in the entire material. The idea developed in this work is to study the contribution of each component.

First of all, a simplified formulation is set up, including a limited number of components (2-3 components for each category as abrasives, lubricants, fillers, reinforcing fibers). Then, a deep bibliographical research is done on the nature of interactions, expected effects of each raw material with the chosen binder (typically a traditional phenolic resin) and which concentration is the most effective for the desired effect. The experimental work starts with the creation of binary system containing only the binder and a filler. Its properties are tested and quantified. Then at the binary system is added another constituent, the properties system are characterized. Step by step the system gets more complex with the systematic characterization of the material properties until the complete formulation material is reached. This way, an evaluation of each filler contribution is performed.

The chosen formula is composed of a binder, a novolac phenolic resin; some reinforcing fibers as aramid and steel; a group of fillers in which are vermiculite, barite, friction dust; and finally as frictional additives graphite, zirconium oxide and aluminium oxide. The binary systems contain only the binder and the aramid fiber in order to give a strong structure to the shaped material. Then the components to create the multiple systems are added in respect to their final content in the formula (excrescent order). The characterization is done using a ball-on-disk.

We have seen in this work a particular way to study components interaction in a brake pad formula. It is obviously only a model proposal, that in the case of a particular mix gives us precious indications in order to improve it and tailor the desired properties of this material modifying the ingredients nature or proportions.

EXPERIMENTAL CHARACTERIZATION AND MODELING OF FRICTION AT THE HEAD/TAPE INTERFACE

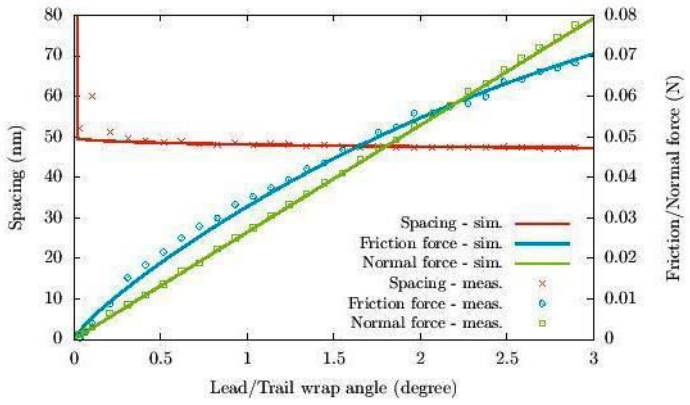
Peter Reininger and Mark A. Lantz

IBM Research – Zurich, CH-8803 Rueschlikon, Switzerland

The explosion in the rate at which digital data is being created is driving demand for cost effective storage technology. Magnetic tape systems are well suited to meet this demand due to their very low total cost of ownership and high reliability. However, in order to remain successful, it is critical to continue to scale the areal density and hence the capacity of tape systems at least as fast as competing technologies.

Magnetic tape systems are somewhat unique in that they use a contact recording technology in which the recording medium is in physical contact with the recording head. In modern tape drives, the tape is wrapped over the head at a small angle of a few degrees and with an applied tension on the order of 1N. The edges of the head are sharp in order to scrape off the air bearing that would otherwise naturally form as the tape is streamed over the head. These results in a low air pressure zone under the tape, that forces the tape into contact with the head and into close proximity to the read and write transducers. However, the spacing between the tape and the head, as well as the friction distribution, are strongly dependent on the actual tape drive parameters, i.e. tape velocity, tension, wrap angle and the used tape media. Controlling friction and wear at the tape/head interface is critical to the recording performance, reliability and lifetime of a magnetic tape system.

In this work we present a model that accurately predicts the friction force at the tape/head interface over the whole range of tape drive parameters. We employ a finite-element model that incorporates the Euler-Bernoulli equation for the mechanical behavior of the tape. The laminar flow between the head and tape is modeled using the Reynolds equation. The contact pressure is modeled empirically using an asperity compliance function, which comprises the relationship between pressure and head/tape spacing. In order verify our model, we measured the head/tape spacing, the friction force and the normal force as a function of the given tape drive parameters. The figure shows one set of data obtained for a flat head operated at a velocity of 4 m/s and a tension of 0.7 N. The simulation accurately predicts the measured values. The difference of the magnetic spacing at very low wrap angles originates from imperfect skiving edge of the measured head.



Comparison of the model and the measurement results of the head/tape spacing, the friction force and the normal force for one set of measurement parameters

[1] Engelen, J. B., & Lantz, M. A. (2015). Asymmetrically Wrapped Flat-Profile Tape–Head Friction and Spacing. Tribology Letters, 59(1), 1-8.

Tuesday 5th, Morning

Session chair: Astrid S. de Wijn

8h50-9h00 Introduction by Nicola Manini

9h00-9h40 Tomas Polcar
Nanoscale friction and wear of solid lubricant coatings

9h40-10h00 Aleksandr Volokitin
Frictional drag force between AFM tip and a graphene-covered plate

10h00-10h20 Eui-Sung Yoon
Polymer pattern geometries for tuning nanofriction

10h20-10h40 Roberto Guerra
Simulating friction of nano-objects

10h40-11h40 Coffee break

11h40-12h20 Maria Clelia Righi
Ab initio investigation of tribochemistry mechanisms in solid and boundary lubrication

12h20-12h40 Elisabetta Serpini
MOS_2 PVD this films: role of physisorbed water on friction and wear

12h40-13h20 Giampaolo Mistura
Thermolubricity and superlubricity of xenon islands

13h20-14h20 Lunch break

NANOSCALE FRICTION AND WEAR OF SOLID LUBRICANT COATINGS

Tomas Polcar

Engineering and the Environment, University of Southampton, Highfield Southampton SO17 1BJ, UK

Atomic Force Microscope is one of very few available tools to bridge the gap between atomistic simulations and macroscopic testing in tribology. In this talk we will briefly discuss some limitations of AFM to be used in Friction Force Mode (FFM), such as a lack of clarity how to derive friction from force measurement and specific problems related to tribocharging. Then we will focus on FFM analysis of novel solid lubricant coatings, in particular formation of an ultrafilm tribolayer and wear at nanoscale. Finally, we will compare FFM results (friction and wear) with data obtained from macroscopic pin-on-disc measurements and relate the results to coating microstructure and mechanical properties.

FRICTIONAL DRAG FORCE BETWEEN AFM TIP AND A GRAPHENE-COVERED PLATE

A. I. Volokitin[1, 2]

[1] Peter Grunberg Institute, Juelich Research Center, Germany
[2] Samara State Technical University, Samara, Russia

At present with new experiments interest is reviving to study the Casimir forces, near-field radiative heat transfer and Casimir friction. The theory of the Casimir friction predicts the friction force between bodies without direct mechanical contact between them when it is associated with the fluctuating electromagnetic field in the vacuum gap between bodies due to the thermal and quantum fluctuations inside the bodies. The noncontact friction is important, for example, for the ultrasensitive force registration because the force fluctuations and friction are linked via the fluctuation-dissipation theorem. The noncontact friction even exists between two absolutely flat surfaces sliding relative to each other at T=0 K when it is associated with relative sliding of quantum fluctuations. While the Casimir force and near-field radiative heat transfer have been measured in many experiments, the detection of the Casimir friction is still challenging problem for experimentalists. However, the frictional drag between quantum wells and graphene sheets, and measurements of the current-voltage dependence of graphene on the polar dielectric substrate SiO_2 were accurately described using the theory of the Casimir friction. In the frictional drag experiment the Casimir friction force between the charge free carriers in the 2D sheets induces the electric field in the sheet, which can be measured. For the graphene sheet situated nearby the polar dielectric substrate the Casimir friction force between the charge free carries in graphene and the surface phonon polaritons in dielectric gives rise to the change of the resistivity of graphene which also can be measured. So far the Casimir friction was detected only using the electrical effects, which it produces. From fundamental point of view and for the applications it is important to study the Casimir friction mechanically by directly measuring the friction force. The possibility to detect the Casimir friction using ARM is discussed. On the AFM tip situated above a graphene-covered plate will act the friction force when the current is induced in the graphene sheet. This friction force will produce the bending of the cantilever, which can be measured. The friction force between the AFM tip and a graphene-covered dielectric is calculated using the fluctuation electrodynamics and studied in the dependence on the separation, the temperature and for the different materials.

[1] A. I. Volokitin and B. N. J. Persson, Influence of electric current on the Casimir forces between graphene sheets, EPL, 103, 24002 (2013)

[2] A. I. Volokitin and B. N. J. Persson, Quantum Friction, Phys.Rev.Lett. 106, 094502 (2011)

POLYMER PATTERN GEOMETRIES FOR TUNING NANOFRICTION

Prashant Pendyala[1], H.S. Grewal[2], H. N. Kim[1], Il-Joo Cho[1] and Eui-Sung Yoon[1]

[1] Center for BioMicrosystems, Brain Science Institute, Korea Institute of Science and Technology
[2] Shiv Nadar University, Gautam Buddha Nagar, Uttar Pradesh, India

At nano scales, the effective range of intermolecular forces is comparable to the dimensions of the interacting asperities. Hence, the geometrical details of the moving contact zone become significantly important. In addition, detailed experimental studies of well-defined nano-contacts can result in a fundamental understanding of friction. In this study, we study the fundamental tribological behavior of geometrically complex polymer nano-pillar surfaces generated using a combination of capillary force lithography and nano-drawing methods. We attempt to deconvolute the individual role of top-surface geometry and the stiffness of the pillars, in overall sliding behavior, using round and flattop, cylindrical and mushroom-like nano pillar surfaces with varying lateral stiffness. Hierarchical patterns containing distributed round-top nano-pillar geometries were used to qualify the role of support systems. Adhesion and frictional behavior of the surfaces was investigated using atomic force microscopy at different relative humidity levels (5% to 80%) and applied normal loads (40 nN to 120 nN). We study the role of intermolecular and capillary forces activated in the confined spaces between the nano-features and the ball, in the overall contact behavior. It is shown that curvature of the pillar asperities significantly influences adhesion and frictional characteristics. For the mushroom-like pillar surfaces, the mechanics of the overhanging flange was the deciding factor. We show that conformability of asperity structure, which controls interaction region, is the principal factor influencing the adhesion and frictional behaviors.

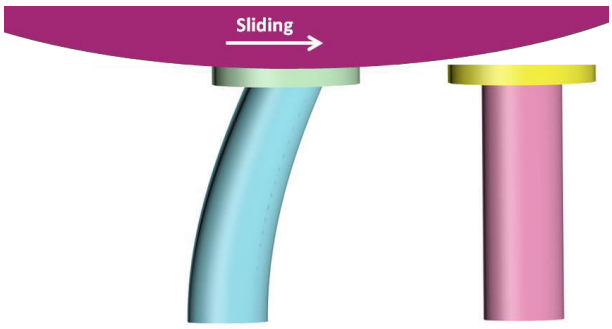


Figure 1: Schematic of an Atomic Force Microscopy spherical indenter sliding on a nano mushroom-like pillar patterned surface

[1] Jeong, Hoon Eui, et al. "Stretched polymer nanohairs by nanodrawing." Nano letters 6.7 (2006): 1508-1513.

[2] Suh, Kahp Y., et al. "Capillarity-assisted fabrication of nanostructures using a less permeable mold for nanotribological applications." Journal of applied physics 100.3 (2006): 034303.

[3] Grewal, H. S., et al. "Nanotribological and wetting performance of hierarchical patterns." Soft matter 12.3 (2016): 859-866.

SIMULATING FRICTION OF NANO-OBJECTS

Roberto Guerra

International School for Advanced Studies - SISSA, Trieste, Italy

The high complexity of dealing with systems with many degrees of freedom under a strict size confinement arises especially in sliding friction phenomena, where the key mechanisms take place at a buried interface. In the last three decades, developments in nanotechnology have extended the experimental study of friction, permitting the analysis on well-characterized materials and surfaces at the nano and mesoscale. Here, by presenting two case studies related to the frictional properties of physisorbed islands [1-3] and nanotubes [4], we show how modelling and molecular dynamics simulations can help in advancing our theoretical understanding in the field of nanotribology.

[1] N. Varini, A. Vanossi, R. Guerra, D. Mandelli, R. Capozza, and E. Tosatti, 'Static friction scaling of physisorbed islands: the key is in the edge', Nanoscale 7, 2093 (2015).

[2] M. Pierno, L. Bruschi, G. Mistura, G. Paolicelli, A. di Bona, S. Valeri, R. Guerra, A. Vanossi, and E. Tosatti, 'Frictional transition from superlubric islands to pinned monolayers', Nature Nanotechnology (2015).

[3] R. Guerra, E. Tosatti, and A. Vanossi, 'Slider Thickness Promotes Lubricity: from 2D Islands to 3D Clusters', Nanoscale 8, 11108 (2016).

[4] I. Leven, R. Guerra, A. Vanossi, E. Tosatti, O. Hod, 'Multi-Walled Nanotube Faceting Unravelled', submitted

AB INITIO INVESTIGATION OF TRIBOCHEMISTRY MECHANISMS IN SOLID AND BOUNDARY LUBRICATION

P. Restuccia[1], S. Lohelè[2], G. Levita[3], S. Kajita[3,4] and M. C. Righi[1,3]

[1] Department of Physics, Informatics and Mathematics, University of Modena and Reggio Emilia
[2] Total Research Center Solaize, France
[3] CNR-Institute of Nanoscience
[4] Toyota Central R&D Labs., Nagakute, Japan

Tribologically-induced chemical modifications of surfaces interacting with lubricant additives or other molecules present in the environment surrounding the sliding media can substantially change the adhesion and friction of materials in contact, therefore it is highly desirable to understand how they take place. However, tribochemical reactions are difficult to monitor in real-time by experiments, which leaves a gap in the atomistic understanding required for their control.

We investigate the tribochemistry of some of the most common solid lubricants, namely molybdenum disulfide, graphene/graphite and carbon-based films, the performances of which are highly affected by humidity. We apply ab initio molecular dynamics to monitor the chemical reactions involving water molecules activated at the sliding interface. Combining the results of the dynamic simulations with thermodynamic analysis based on static first principles calculations, we elucidate important differences in the tribochemistry of the considered layered materials [1]. We explain the effects of Si dopants in enhancing the hydrophilic character of carbon-based films and discuss its impact on the sliding properties [2, 3].

As second issue, we investigate the tribochemistry of sulfur-, phosphorus-containing additives and graphene at iron interfaces.[4,5,6] The results point at the important role of metal passivation in reducing the adhesion and shear strength of the interface. We generalize the result by establishing a connection between the tribological and the electronic properties of interfaces. This adds a new piece of information for the ultimate understanding of the fundamental nature of frictional forces.

[1] P. Restuccia, G. Levita and M. C. Righi Understanding the tribochemistry of graphene and molybdenum disulfide interacting with water by ab initio molecular dynamics. To be published.

[2] S. Kajita and M. C. Righi Insights into the tribochemistry of silicon-doped carbon based films by ab initio analysis of water/surface interactions, Tribology Letters, 61,17 (2016)

[3] S. Kajita and M. C. Righi A fundamental mechanism for carbon-film lubricity identified by means of ab initio molecular dynamics, Carbon 103, 193 (2016)

[4] M. C. Righi, S. Loehle', M. I. de Barros Bouchet, D. Philippon and J. M. Martin Trimethyl-phosphite dissociative adsorption on iron by combined first-principle calculations and XPS experiments, RSC Advances 5, 101162 (2015)

[5] M. I. de Barros Bouchet, M. C. Righi, D. Philippon, S. Mambingo-Doumbe, T. Le-Mogne, J. M. Martin and A. Bouffet Tribochemistry of phosphorus additives: experiments and first-principles calculations, RSC Advances 5, 49270 (2015)

[6] P. Restuccia and M. C. Righi Tribochemistry of steel lubrication by graphene. Submitted (2016)

MOS_2 PVD THIN FILMS: ROLE OF PHYSISORBED WATER ON FRICTION AND WEAR

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Molybdenum disulphide (MoS_2) is a well-known solid lubricant that has been used since the Sixties in aerospace applications due to its extremely low coefficient of friction (0.01-0.04) in high vacuum. In these applications, solid lubricant coatings are usually in the thickness range between 100 and 500 nm because of the optimized precision tolerances required [1]. Among the many existing deposition techniques, PVD magnetron-sputtering offers the greatest potential for custom tailoring thin lubricating coatings with the desired morphological and tribological properties [1, 7]. In the last twenty years, efforts have been made to improve the tribological performances of MoS_2-based coatings in ambient environment [2]. Even if there is an extensive literature dealing with the causes of failure of MoS_2 in humid environment, a general agreement on the prevailing mechanism, surface oxidation or water molecules physisorption, is still lacking, and conflicting studies have been published over the years [3-7].

We report on MoS_2 thin (200 nm) coatings deposited on Si (111) single crystal in Ar_+ atmosphere by RF magnetron sputtering. Composition and morphology of the coatings were investigated by means of Scanning Electron Microscopy (SEM), Auger Electron Spectroscopy (AES) and Focused Ion Beam (FIB). Surface morphology was checked via AFM. Silicon single crystal was chosen because it offers a very flat surface. In this way we are able to minimize the role of surface to the tribological behavior of MoS_2. It represents also the most used material in MEMS and NEMS. Pin-on-disc tests show a reduction of friction coefficient in different atmospheres with respect to humid air. The counterpart was a 4 mm 100Cr6 steel ball, while the different atmospheres chosen were dry air, nitrogen and oxygen. The extent of the friction coefficient reduction depends mostly on the overall level of humidity and on sample temperature. Pump and purge experiments and an accurate chemical analysis reinforce the conclusion that the prevailing phenomenology is linked to environmental humidity, and not to oxidation. To further validate our results, AFM friction measurements on exfoliated MoS_2 single crystal were performed.

The authors would like to acknowledge support from COST action MP1303.

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[7] T. W. Scharf, S. V. Prasad, J Mater Sci 48, 511 (2013)

THERMOLUBRICITY AND SUPERLUBRICITY OF XENON ISLANDS

Giampaolo Mistura, Matteo Pierno and Lorenzo Bruschi

Dipartimento di Fisica e Astronomia G. Galilei, Università di Padova, via Marzolo 8, 35131 Padova, Italy

We present the results of recent quartz crystal microbalance (QCM) studies of the sliding frictionof Xe islands on graphene [1] and on Cu(111) [2]. Nanofriction of Xe monolayers deposited on graphene is investigated at temperatures between 25 and 50 K. At low temperatures, the Xe monolayers are fully pinned to the graphene surface. Above 30 K, the Xe film slides and the depinning onset coverage beyond which the film starts sliding decreases with temperature. In the case of Xe on Cu(111), QCM data show remarkably large slip times at increasing submonolayer coverages, signaling superlubricity, followed by a dramatic drop to zero for the dense commensurate monolayer.

[1] M. Pierno, L. Bignardi, M.C. Righi, L. Bruschi, S. Gottardi, M. Stohr, O. Ivashenko, P.L. Silvestrelli, P. Rudolf and G. Mistura, Thermolubricity of gas monolayers on graphene, Nanoscale 6, 8062-8067 (2014)

[2] M. Pierno, L. Bruschi, G. Mistura, G. Paolicelli, A. di Bona, S. Valeri, R. Guerra, A. Vanossi and E. Tosatti, Frictional transition from superlubric islands to pinned monolayers, Nature Nanotechnology 10, 714-718 (2015)

Tuesday 5th, Afternoon

Session chair: Karine Mougin

14h20-15h00 Graham Leggett
Contact mechanics and thermodynamics in sliding contacts between molecular materials

15h00-15h20 Thilo Glatzel
Adsorption properties of isolated porphyrine molecules on TiO_2

15h20-15h40 Oguzhan Gurlu
Identification of subsurface and interface defects with friction force microscopy

15h40-16h20 Jacqueline Krim
Controlling friction with external electromagnetism

16h20-18h40 Poster Cession and Coffee break

19h00-20h00 MC Meeting

CONTACT MECHANICS AND THERMODYNAMICS IN SLIDING CONTACTS BETWEEN MOLECULAR MATERIALS

Graham Leggett

Department of Chemistry, University of Sheffield, Brook Hill, Sheffield S3 7HF

The atomic force microscope (AFM) has been used widely to study nanoscale tribological phenomena, but a unified model for the mechanics of the tip-sample interaction has been lacking. Experimental data show that nanoscale friction depends strongly on interfacial chemistry, but these correlations have not been explained adequately by existing models. Recent measurements of interactions between hydrogen bond-forming molecules adsorbed onto solid surfaces and AFM tips shed new light on this problem. By making measurements in liquid mixtures, a quantitative correlation has been found between the surface shear strength in a nanoscale contact and the free energy of solution-phase hydrogen bonding interactions, uniting classical contact mechanics with equilibrium thermodynamics. The thermodynamics of intermolecular interactions may be determined quantitatively from nanoscale friction measurements. The contact mechanics are best modeled by treating the friction force as the sum of a load-dependent term (attributed to "molecular plowing") and an area-dependent term attributed to shearing (adhesion). The relative contributions of plowing and shearing are determined by the coefficient of friction, μ, and the surface shear strength τ. The transition from adhesion- to load-determined friction is controlled by the solvation state of the surface: solvated surfaces represent a limiting case in which the shear term approaches zero, and the friction-load relationship is linear, while in other circumstances, the friction-load relationship is non-linear and consistent with Derjaguin-Muller-Toporov (DMT) mechanics. The approach has been extended to hydrocarbon surfaces. While for these systems the adhesive interaction may be modeled using the Lifshitz theory, the friction still separates into an adhesion-independent load-dependent term and an adhesion-controlled area-dependent term; the value of μ is found to be independent of the adhesion force.

For polymer brush systems the mechanics are more complex, because of the small stiffness of swollen brushes. Nevertheless, the friction can still be treated as the sum of a load-dependent plowing term and an adhesion-controlled shear term. The shear term is sensitive to polymer solvation: where the brush is strongly solvated, the adhesion is negligible and plowing provides the main dissipative pathway. For collapsed brushes in a poor solvent, plowing also dominates. However, for intermediate degrees of solvation, a range of behavior is observed that correlates with the solvent strength. The importance of brush morphology in determining nanometer-scale friction has been explored in a variety of ways. Using near-field lithography, structures of varying density may be fabricated by using the local probe to selectively deprotect an aminosiloxane film functionalized by a photocleavable nitrophenyl protecting group. After deprotection, the amine groups are functionalized with an initiator for atom transfer radical polymerization (ATRP) and brushes are grown. By varying the writing rate, the brush density can be controlled. The correlation between surface friction and brush density can be studied quantitatively. Alternatively, interferometric lithography of a brominated siloxane film has been used to fabricate nanostructured brushes over large areas. Exposure of the brominated adsorbate in the interferometer leads to selective removal of the Br initiator form the surface; by controlling the exposure, the density of Br and the dimensions of the features may be controlled so that brushes of controlled morphology are grown subsequently from the patterned surface by ATRP. The resulting structures enable the correlation between contact mechanics and brush morphology to be explored quantitatively.

ADSORPTION PROPERTIES OF ISOLATED PORPHYRINE MOLECULES ON TIO_2

R. Jöhr[1], A. Hinaut[1], R. Pawlak[1], A. Sadeghi[2], S. Goedecker[1], P. Olszowski[3], L. Zając[3], S. Godlewski[3], B. Such[3], M. Szymonski[3], E. Meyer[1] and Th. Glatzel[1]

[1] University of Basel, Department of Physics, Basel, CH-4056, Switzerland
[2] Shahid Beheshti University, Physics Department, IR-19839, Tehran, Iran
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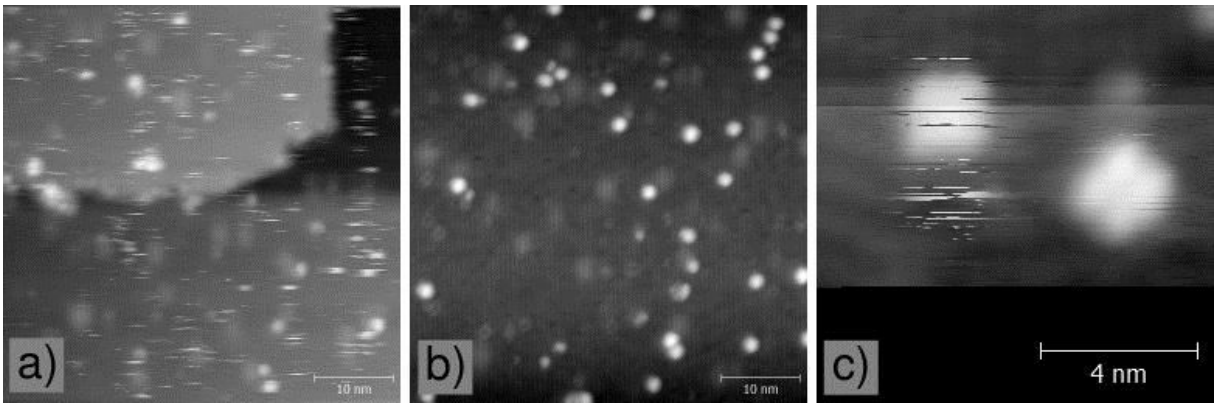
Titania surfaces sensitized with metallo-porphyrins are of increasing interest for photocatalysis or photovoltaics [1]. In these applications, the dye absorbs light and injects the exited electron into the conduction band of the titania. The binding configuration is thereby of great importance for the electron transfer process. To simultaneously investigate the binding configuration and its influence on the charge transfer process, non-contact Atomic Force Microscopy (nc-AFM) and in particular Kelvin Probe Force Microscopy (KPFM) are the methods of choice.

In our work we studied the adsorption properties of isolated porphyrin molecules containing a different number (0-4) of carboxyphenyl groups changing the adsorption behavior on anatase and rutile TiO_2. Bimodal nc-AFM at room temperature and under ultrahigh vacuum (UHV) was applied to obtain high resolution on the molecules as well as on the substrate. The experimental data reveals that the porphyrin molecules align themselves with respect to the substrate structure resulting in well-defined orientations [2, 3]. The number of carboxyl groups, the preparation temperature, and the configuration of surface adsorbates are responsible for the binding strength of the molecules. Figure a) shows stable as well as mobile porphyrine molecules with two carboxylic groups in trans configuration on a TiO_2 surface, after annealing at 300°C for 30min (Fig b)) all of the molecules are stabilized. High resolution measurement of similar molecules in cis configuration (Fig c)) revel the detailed absorption configuration in dependence on the mobility. Results from DFT calculations using the deduced binding configurations as input were in good agreement with the experimental data.



nc-AFM images of zinc porphyrine molecules with two carboxyl groups in trans configuration on a TiO_2 surface. a) directly after deposition, b) after annealing at 300°C for 30min, and c) porphyrines in cis configuration and with high resolution.

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[2] P. Olszowski et al., JPCC, 119, 21561, (2015)

[3] R. Jöhr et al., JCP, 143, 094202, (2015)

IDENTIFICATION OF SUBSURFACE AND INTERFACE DEFECTS WITH FRICTION FORCE MICROSCOPY

Oğuzhan Gürlü[1], Umut Kamber[1], Cem Kıncal[1], Dilek Yıldız[2], Clara Grygiel[3] and Cornelis J. Van Der Beek[4]

[1] Istanbul Technical University, Istanbul, Turkey
[2] University of Basel, Basel, Switzerland
[3] Université de Caen, Caen, France
[4] Ecole Polytechnique, Palaiseau, France

Formation of Swift Heavy Ion (SHI) induced defects on Highly Oriented Pyrolytic (HOPG) surfaces were reported in numerous studies. Hillock-like and comet-like structures have been observed with STM. We employed Friction Force Microscopy (FFM) in order to study the effects of SHIs on the sub-surface region of the HOPG crystals. Here we report that, comet-like structures on HOPG formed due to SHI irradiation under grazing incidence can be imaged by both STM and FFM. Our STM data showed that atomic resolution could be achieved on the tail section of the comet like structures. This proved that, while the SHI travelled in the bulk of the crystal, it did not destroy the surface, yet the interaction of the SHI with the bulk appeared as a height difference on the surface when imaged by STM. FFM measurements showed complementary results to our STM measurements with further details. We observed that the tails of the comet-like structures appeared on the friction map, although they could not be seen in the AFM topography maps. These results may answer the origin of the tail section of the comet-like structures forming in grazing incidence SHI experiments.

FFM was applied in the identification of the impurities on surfaces in another complementary study: By changing the conditions of CVD process for graphene growth, we discovered a way to produce dendritic silicon-oxide structures. Such structures were observed both on graphene/Cu-foil system and on pure Cu-foils after CVD process. We investigated whether these structures formed on or under the graphene on copper foils by investigating the friction properties of such surfaces near and on dendrites forming on graphene grown copper surfaces. We also performed FFM measurements on silicon-oxide structures forming on bare Cu-foils. Comparative data showed that these structures can form both in-between graphene and Cu surface as well as on graphene on copper. We further investigated the potential reasons of such formations in view of the mobility of the silicon species at the graphene-copper interface.

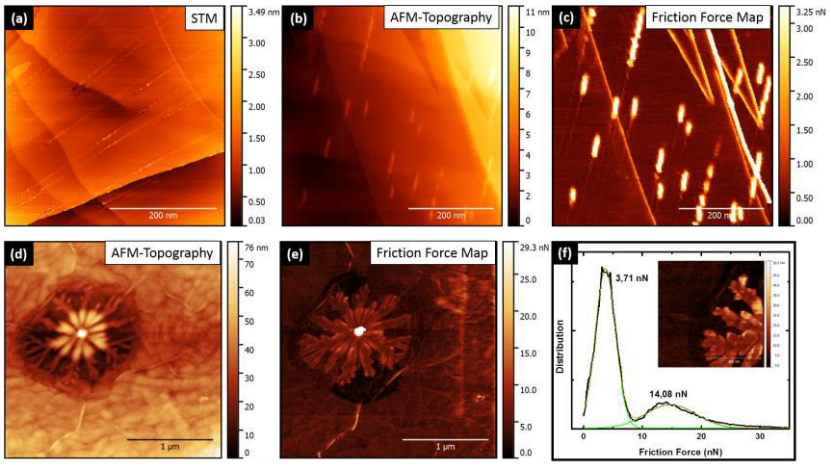

Figure (a) STM topography of SHI irradiated HOPG under grazing incidence, (b) AFM topography of the same sample, (c) Friction Force map of same area with (b). (d) AFM topography of a silicon-oxide dendrite on graphene/Cu-foil, (e) Friction Force map of same area in (d), (f) Friction Force distribution of the scanning area shown in the inset image

CONTROLLING FRICTION WITH EXTERNAL ELECTROMAGNETISM

Jacqueline Krim

Physics Department, North Carolina State University, Raleigh, North Carolina 27695-8202

Studies of the fundamental origins of friction have undergone rapid progress in recent years, including measurements of the sliding friction of physisorbed monolayers and bilayers in gaseous and liquid environments by means of a quartz microbalance technique [1]. These measurements have in the past provided information on the relative contributions of electronic, magnetic, electrostatic and phononic dissipative mechanisms. They are now evolving into methods that allowing external control of nano and/or meso scale friction through tuning of magnetic and electric fields external to the contact.

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Wednesday 6th, Morning

Session chair: Nicola Manini

8h50-9h00 Introduction by Nicola Manini

9h00-9h40 Ruben Perez
Atomic-scale sliding friction on graphene in water

9h40-10h00 Michael Urbakh
Frictional properties of nanojunctions including atomically thin sheets

10h00-10h20 Rosario Capozza
Shear induced structural rearrangements in molebdenum disulfide studied by molecular dynamic simulations

10h20-10h40 Ion Marius Sivebæk
Shearing nanometer-thick confined hydrocarbon films: Friction and adhesion

10h40-11h40 Coffee break

11h40-12h20 Alessandro Siria
Solid-Solid and Liquid-Solid friction in individual nanotubes

12h20-12h40 Jean Comtet
Electrically-induced solidification of confined ionic liquids

12h40-13h00 Marcin Kisiel
Elasticity study of the polymer surface by oscillating contact of atomic force microscope

13h00-13h20 Filippo Federici Canova
Machine learning approach for lubricant optimisation

13h20-14h20 Lunch break

ATOMIC-SCALE SLIDING FRICTION ON GRAPHENE IN WATER

J. G. Vilhena[1,2], Carlos Pimentel[3,4], Patricia Pedraz[5], Feng Luo[5], Pedro A. Serena[2], Carlos Pina[3,4], Enrico Gnecco[5,6] and Rubén Pérez[1,7]*

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[2] Instituto de Ciencia de Materiales de Madrid (ICMM), Madrid, Spain
[3] Universidad Complutense de Madrid, Madrid, Spain
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[5] Instituto Madrileño de Estudios Avanzados (IMDEA), Madrid, Spain
[6] Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Jena, Germany
[7] Condensed Matter Physics Center (IFIMAC), Universidad Autonoma de Madrid, Madrid, Spain
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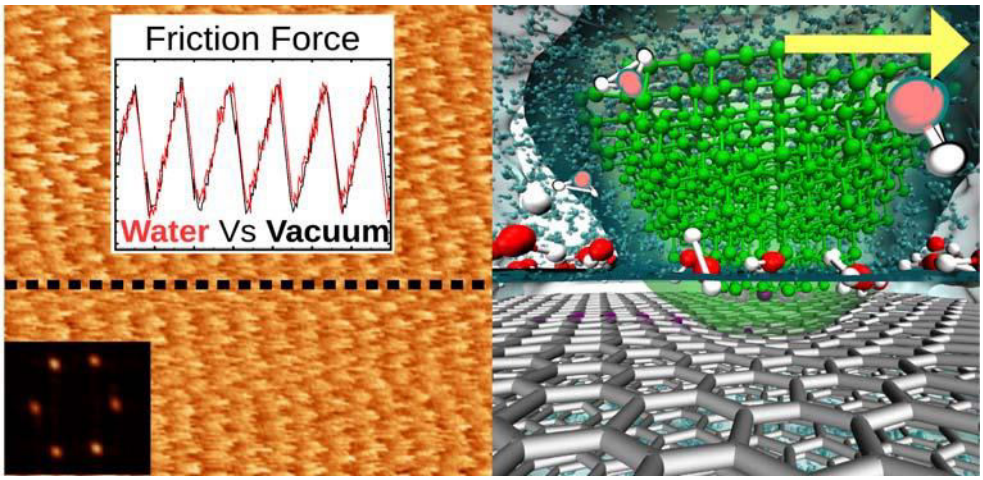
The sliding of a sharp nanotip on graphene completely immersed in water is investigated by molecular dynamics (MD) and atomic force microscopy [1]. MD simulations predict that the atomic-scale stick-slip is almost identical to the one found in ultra-high vacuum. Furthermore, they show that water plays a purely stochastic role on sliding (solid-to-solid) friction. These observations are substantiated by friction measurements on graphene grown on Cu and Ni, where, oppositely to operation in air, lattice resolution is readily achieved. Our results not only promote friction force microscopy in water as a robust alternative to ultra-high vacuum measurements but also they suggest that friction measurements could unveil the subtle dynamical lateral order induced by a hydrophobic material like graphene on the water hydration layer. Finally, we shall explore the influence of substrate morphology, particularly the presence of steps, on friction and the sliding properties of biological material on a hydrophobic surface as graphene under physiological conditions.



(Left) FFM image of graphene as measured in water highlighting the lattice resolution. (inset) friction force obtained from MD simulations at a normal load of 20 nN in vacuum and water. (Right) Atomistic representation of FFM embedded in water (tip atoms (green), graphene (dark grey), water molecules close to the tip are highlighted (O, red; H, white))

[1] J. G. Vilhena, Carlos Pimentel, Patricia Pedraz, Feng Luo, Pedro A. Serena, Carlos Pina, Enrico Gnecco, and Rubén Pérez, ACS Nano (2016) DOI: 10.1021/acsnano.5b07825

FRICTIONAL PROPERTIES OF NANOJUNCTIONS INCLUDING ATOMICALLY THIN SHEETS

Wengen Ouyang[1], Ming Ma[2], Quanshui Zheng[1] and Michael Urbakh[2]

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Using nonequilibrium molecular dynamics simulations and a coarse-grained description of a system, we have investigated frictional properties of nanojunctions including atomically thin sheets embedded between metal surfaces. We found that the frictional properties of the junctions are determined by the interplay between the lattice mismatch of the contacting surfaces and out-of-plane displacements of the sheet. The simulations provide insight into how and why the frictional characteristics of the nanojunctions are affected by the commensurate−incommensurate transition. We demonstrated that in order to achieve a superlow friction, the graphene sheet should be grown on or transferred to the surface with morphology, which is close to that of the graphene (for instance, Cu), while the second confining surface should be incommensurate with the graphene (e.g., Au). Our results suggest an avenue for controlling nanoscale friction in layered materials and provide insights in the design of heterojunctions for nanomechanical applications.

SHEAR INDUCED STRUCTURAL REARRANGEMENTS IN MOLYBDENUM DISULFIDE STUDIED BY MOLECULAR DYNAMICS SIMULATIONS

Paolo Nicolini[1] and Rosario Capozza[2]

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[2] Italian Institute of Technology-IIT, Via Morego 30, 16163 Genova, ITALY

Molybdenum disulfide, the most studied member of the transition metal dichalcogenides family, has been used as solid lubricant for several decades, showing extremely low friction coefficients [1] and stability to high temperature. Its lubricating properties are ascribed to the weak van der Waals interactions between sulfur atoms in the crystalline layered structure. Moreover MoS_2, even when prepared in the amorphous state or made of randomly oriented domains, can undergo shear induced structural transitions to the more ordered layered state affecting its tribological properties [2].

Exploiting a recently developed classical force field [3] able to treat explicitly formation and breaking of bonds, we investigate by molecular dynamics simulations, the shear induced structural changes and possible layer formation in the amorphous molybdenum disulfide. Tribological properties are also monitored during the simulations and studied against the effect of load, velocity and temperature.

This study aims at gaining an atomic level understanding of the dynamics of layer formation process in MoS_2 controlling and possibly improving its tribological properties.

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SHEARING NANOMETER-THICK CONFINED HYDROCARBON FILMS: FRICTION AND ADHESION

Ion M. Sivebaek[1,2,3] and Bo N.J. Persson[1]

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[2] Novo Nordisk A/S, Device R&D, DK-3400 Hillerod, Denmark
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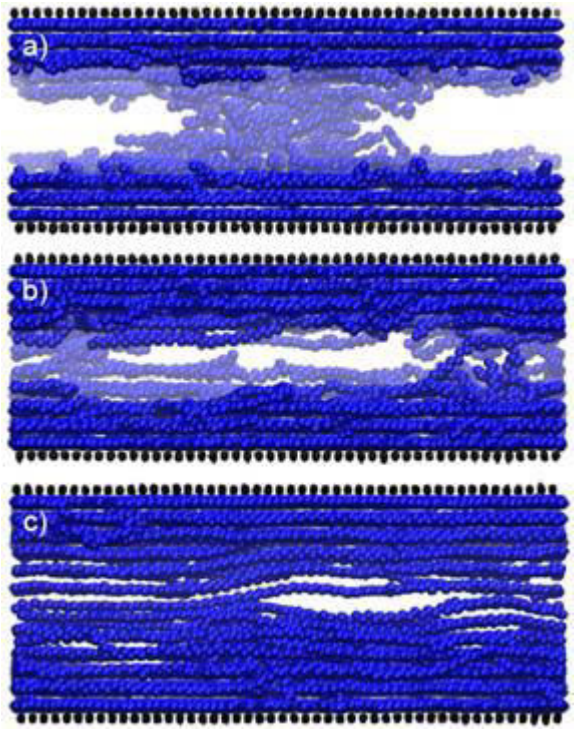
We present Molecular Dynamics (MD) friction and adhesion calculations for nanometer-thick confined hydrocarbon films with molecular lengths 20, 100 and 1400 carbon atoms [1]. We study the dependency of the frictional shear stress on the confining pressure and sliding speed [1-3]. We present results for the pull-off force as a function of the pull-off speed and the sliding speed. Some of the results are analysed using the simple cobblestone model and good semi-quantitative agreement between the model predictions and the MD results are found [4].

The figure shows snapshots of the films of hydrocarbons of different lengths while there is both sliding and pull-off. It can be observed that the shortest molecules form capillary bridges whereas the longest ones have a well-defined interface in the middle of the film. We will show the importance of this for practical applications e.g. medical devices.



Snapshots of the films of a) $C_{20}H_{42}$, b) $C_{100}H_{202}$ and c) $C_{1400}H_{2802}$. The sliding velocities are 100 m/s and 1 m/s in the x and z directions respectively. The surfaces have been separated by about 2 nm.

[1] I. M. Sivebaek, V. N. Samoilov, and B. N. J. Persson, “Frictional properties of confined polymers,” Eur. Phys. J. E, vol. 27, no. 1, pp. 37–46, 2008.

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[4] I. M. Sivebaek and B. N. J. Persson, “Shearing Nanometer-Thick Confined Hydrocarbon Films: Friction and Adhesion,” Tribol. Lett., vol. 62, no. 1, p. 5, 2016.

SOLID-SOLID AND LIQUID-SOLID FRICTION IN INDIVIDUAL NANOTUBES

Alessandro Siria, Eleonora Secchi, Antoine Niguès, Sophie Marbach and Lyderic Bocquet

Laboratoire de Physique Statistique de l'Ecole Normale Supérieure, 24 rue Lhomond 75005 Paris, France

Individual Nanotubes are ideal candidates to study the fundamental origin of friction at nanoscale. They exhibit a perfectly flat surface with a controlled crystallinity and well specified interaction between the surface material. They present concentric crystalline layers which can slide against each other with pure one dimensional directional motion; further they allow to confine water inside atomically pristine nanoscale pipes. They are indeed the ideal system to explore the fundamental aspects of solid-solid and liquid-solid friction. In this talk we present an experimental study of interlayer solid friction and fluid solid friction inside Carbon and Boron Nitride nanotubes (CNT and BNNT). CNT and BNNT present the same exact crystallinity but radically different electronic properties. We will show how this difference is at the origin of an opposite behavior for friction [1, 2].

[1] A. Niguès, A. Siria, P. Vincent, P. Poncharal, L. Bocquet, Nature Materials 13 (7) 688-693 (2014)

[2] E. Secchi, S; Marbach, A. Niguès, D. Stein, A. Siria, L. Bocquet, Submitted (2016)

ELECTRICALLY-INDUCED SOLIDIFICATION OF CONFINED IONIC LIQUIDS

Jean Comtet, Antoine Niguès, Lydéric Bocquet and Alessandro Siria*

Laboratoire de Physique Statistique de l'Ecole Normale Supérieure, UMR 8550, 24 Rue Lhomond 75005 Paris, France. *email: alessandro.siria@lps.ens.fr

Using a quartz-tuning-fork-based Atomic Force Microscope [1], we investigate the behavior under confinement and electric field of Bmim-based ionic liquids. We impose subnanometric oscillations of a tungsten AFM tip at a frequency around 32 kHz, and take advantage of the dynamic frequency modulation mode to disentangle conservative (elastic) and dissipative (friction-related) response in the liquid (Fig. 1). Using metallic susbtrates allows us to bias the substrate with respect to the tip and induce controlled electric field in the confined fluid. Using rheological measurements, we show that upon confinement (of the order of tens of nanometers), the liquid adopts a solid-like response, strongly dependent on the applied electric fields. Our results challenge the classical view of ionic liquids and we put them in perspective with recent AFM and SFA friction measurements on ionic liquids in electrochemical cells.

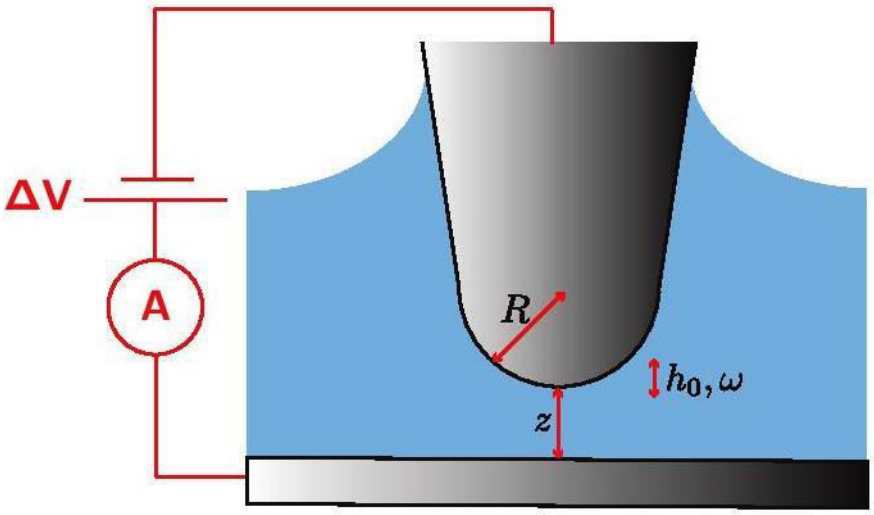

Fig. 1. Schematic of the setup. The AFM tip of end radius R ≈ 1 μm is oscillating at a frequency ω/2π ≈ 32 k[1] A. Niguès, A. Siria, P. Vincent, P. Poncharal, and L Bocquet. Ultrahigh interlayer friction in multiwalled boron nitride nanotubes. Nature materials, 13(7):688–93, jul 2014.

ELASTICITY STUDY OF THE POLYMER SURFACE BY OSCILLATING CONTACT OF ATOMIC FORCE MICROSCOPE

M. Kisiel, A. Bubendorf, Th. Glatzel and E. Meyer

Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

Rapid development of the micro- and nanoscale electromechanical systems (MEMS and NEMS) entails establishing of novel methods for mechanical characterization of materials with high resolution. Nanocomposites and block copolymers are typical examples of those samples, where elasticity spatial distribution resembles the phase separation. The regions of different microphases form nanometer sized structures. Owing to their shape and size, AFM cantilever tips are well-suited to perform measurements with nanometer resolution and hence determine locally the Young modulus. The elasticity of different polymers (PS, PP, LLDPE, Teflon) has been investigated by means of AFM (Atomic Force Microscope) under ambient temperature and in non-dry air. We present here the contact variation of the method developed by Herruzo and Garcia [1]. The approach bases on Phase Lock Loop (PLL) tracking of first two flexural modes of the oscillating cantilever operated in contact regime. The method is very fast and less invasive as compared to standard indentation measurements. It however requires the prior calibration measurements on samples of defined stiffness. We showed that E-modulus might be quantitatively determined for variety of polymers.

[1] E. T. Herruzo, A. P. Perrino, R. Garcia, Nat. Commun.5, 3126 (2014)

MACHINE LEARNING APPROACH FOR LUBRICANT OPTIMISATION

Filippo Federici Canova[1,3], Martha Arbayani Zaidan[1], Adam S. Foster[2] and Lasse Laurson[2]

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[3] Nanolayers Research Computing LTD, United Kingdom

Friction and wear are the main source of failure for any kind of machinery, and can significantly impact the GDP of any industrialised country [1]. As technology scales down towards micro- and nano-mechanical systems, the detrimental effects of friction can seriously hamper the functionality of these devices. Searching for an appropriate lubricant is often a daunting task, due to the wide range of possible chemical compounds, and the cost of evaluating each candidate experimentally. Being able to predict the viscous properties of a lubricant could make the screening process of materials much faster and efficient, however, the relationship between the atomic details of a fluid, and its physical properties, which intuitively exist, is not known. Machine-learning methods were recently applied to physics and chemistry problems [2]. The main idea is to *train* a model to reproduce a database of descriptor-property set for several known systems, feed in a descriptor for a new system predict its properties (Fig. 1). Here we show our experience with machine-learning on lubricant performance. Due to the lack of consistent and sufficient experimental data, we calculated a minimal database of toy-model fluids with classical molecular dynamics. The fluids consist of mixtures of chain-like molecules, nano-confined between atomically flat surfaces. Lubrication performance is quantified by applying a constant shear force to the surfaces and measuring their average shear rate. Simple Lennard-Jones and Morse potentials are used to represent all atomic interactions in the systems. 8000 random mixtures as well as pure liquids of varying chain length (Fig. 2) were calculated. We developed a variety of methods capable of modelling the relationship between viscosity of liquids and their molecular structure. Finally, we found out that a combination of simple neural networks is necessary to accurately fit our ill-behaved data, however, the method is limited to simple descriptors for chains. A more general method [3], capable of describing any chemical system was developed, however a sufficient amount of training data cannot even be computed with molecular dynamics, but we hope it will be useful in the future.

Figure 1: Training and prediction of physical quantities using machine learning methods

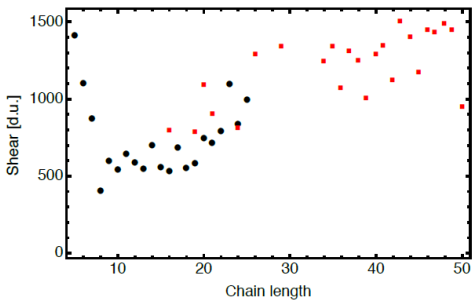


Figure 2: Calculated shear performance of toy liquids of different size

[1] R. W. Carpick, Science, 313, 184 (2006)

[2] M. Rupp, Int. J. Quantum Chem., 115, 1058 (2015)

[3] F. Scarselli, et al., Neural Networks, 20, 61, (2008)

Thursday 7th

Session chair: Sergei Vlassov

9h50-10h00 Introduction by WG4 leader

10h00-10h40 André Schirmeisen
Superlubric sliding nanoparticles: Area scaling, Break-down and ageing dynamics

10h40-11h00 Dirk Dietzel
Contact ageing dynamics analyzed by temperature dependent “slide hold slide” measurements

11h00-11h20 Astrid S. De Wijn
Imagining high-speed friction at the nanometer scale

11h20-12h20 Coffee break

12h20-13h00 Janet Wong
Lubricant flow in an elastohydrodynamic contact

13h00-13h20 Karine Mougin
Manipulation of gold functionalized nanoparticles on flat substrates using a frequency transducer coupled to AFM

13h20-13h40 Closing remarks

SUPERLUBRIC SLIDING NANOPARTICLES: AREA SCALING, BREAK-DOWN AND AGEING DYNAMICS

André Schirmeisen

Institute of Applied Physics (IAP), Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

In an effort to reduce the friction between sliding components scientists and engineers have developed a multitude of lubrication schemes. In the field of dry lubrication the idea of superlubricity, i.e. the state of (almost) vanishing friction, has received widespread attention lately. One of the most intriguing concepts in this framework is referred to as `structural superlubricity', where flat surfaces are thought to slide past each other virtually frictionless if their atomic structures are incommensurate. In this talk, we analyze the fundamental mechanisms that govern the area-dependence of friction in extended but atomically flat contacts of dissimilar materials. The resulting sublinear power laws, which link mesoscopic friction to atomic principles, are then confirmed by measuring the sliding resistance of gold and antimony particles on graphite [1]. On one hand these findings suggest that engineering surfaces with very low friction can be realized up to mesoscopic contact areas. Furthermore, it is shown that nanoparticles can even co-exist in two frictional states, exhibiting 'frictional duality': Some particles show linear scaling with contact area reminiscent of Amonton's friction law while others remain in the superlow friction state of structural lubricity [2]. This duality phenomenon is explained by a model of partial interface contamination. Another limit of superlubricity is dictated by the interaction strength at the particle substrate interface. We have tuned this interaction by alternating the substrate from graphite to MoS_2. On MoS_2 we observed the break-down of superlubricity due to the enhanced chemical Sb-S interaction. Lastly, we investigated the effect of contact ageing, detrimental in the field of earthquake modelling: The shear strength of tectonic plates is believed to increase logarithmic in time, leading to the infamous strong sudden energy dissipation events, i.e. earthquakes. Interestingly, we find that similar ageing dynamics exist for nanoparticles, as evidenced by stick-slip movements of those objects. A complex interplay of ageing dynamics with thermally activated stick-slip friction explains the commonly observed friction peak at low temperatures [3]. These examples demonstrate how nanoparticle manipulation by atomic force microscopy techniques can contribute to the understanding of fundamental friction processes of atomically defined interfaces [4].

[1] D. Dietzel et al., Physical Review Letters 111, 235502 (2013)

[2] D. Dietzel et al., Physical Review Letters 101, 125505 (2008)

[3] M. Feldmann et al., Physical Review Letters 112, 155503 (2014)

[4] D. Dietzel, U.D. Schwarz and A. Schirmeisen, Friction2, 114 (2014)

CONTACT AGEING DYNAMICS ANALYZED BY TEMPERATURE DEPENDENT "SLIDE HOLD SLIDE" MEASUREMENTS

Matthias Vorholzer, Dirk Dietzel and Andre Schirmeisen

Institute of Applied Physics, Justus Liebig University Giessen, Germany

Despite the many advances in recent years in understanding tribological processes at the nanometer scale, the problem of nanoscale contact ageing still remains largely unexplored. Recently, single-asperity slide-hold-slide experiments have been conducted with an AFM at room temperature under ambient conditions to directly investigate the evolution of static friction with time for a standard Si tip sliding on a Si wafer [1]. These results can be explained based on a model that assumes the formation of chemical bonds between the surfaces [2].

The bond formation can be expected to be a thermally activated process and interface temperature is thus expected to play a major role for this ageing process. To verify this assumption, we have now analysed contact ageing as a function of temperature (15K<T<350K) for this material combination under UHV conditions. Independent of the interface temperature our results confirm the logarithmic increase of static friction with increasing hold-time. However, the distinct temperature dependence (Fig. 1) cannot be explained by purely thermally activated processes, but instead suggests that additional processes like viscoelastic contact area variations or the influence of wear need to be considered. To distinguish the different ageing mechanisms, our analysis of the technologically relevant material combination formed by Si tips sliding on Si-wafers will be complemented by additional material combinations, thereby allowing to identify the role of different ageing processes.

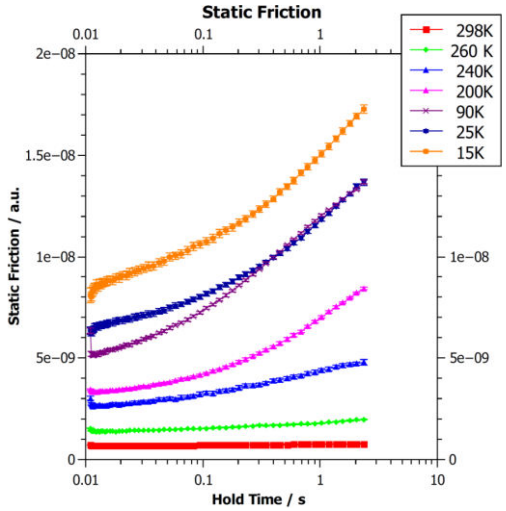


Fig. 1) Static friction as a function of the hold time measured for a Si cantilever on a Si wafer for different temperatures

[1] Li et al., Nature 480, 233-235 (2012)

[2] Liu et al. PRL 109, 186102 (2012)

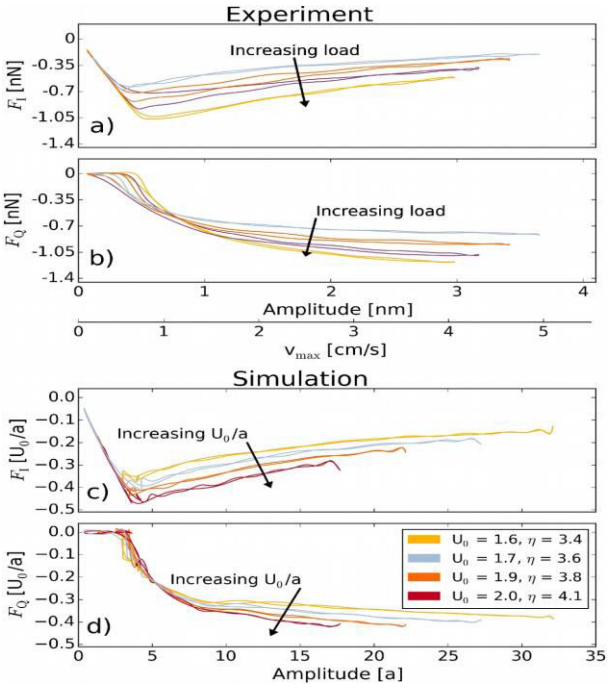
IMAGINING HIGH-SPEED FRICTION AT THE NANOMETER SCALE

Per-Anders Thoren[1], Astrid S. de Wijn[2,3], Riccardo Borgani[1], Daniel Forcheimer[1] and David B. Haviland[1]

[1] Royal Institute of Technology (KTH), Stockholm, Sweden
[2] Stockholm University, Stockholm, Sweden
[3] Norwegian University of Science and Technology, Norway

Real, macroscopic, contacts typically operate at speeds of mm/s or above. Simulations of sliding contacts are also limited to such high speeds for numerical reasons. While we know that understanding what happens at nano scales, currently experimental methods are still lacking that can simultaneously probe forces with nm scale resolution and realistically high velocities. We present a technique[1] for measuring *in detail* the velocity-dependence of frictional forces on an AFM tip reaching velocities up to several cm/s. The method is based on the measurement and analysis of intermodulation products, or frequency mixing of multiple drive tones near a high Q torsional resonance, that are due to the nonlinear frictional force. The method gives the oscillation amplitude dependence of both conservative and dissipative dynamic force quadratures, revealing a transition between stick-slip and smooth sliding that is characteristic of friction at high speeds. We can explain the measurements with a modified Prandtl-Tomlinson model that accounts for the viscous and elastic nature of the asperity. With its high force sensitivity for small sliding amplitude, our method enables rapid and detailed surface mapping of the full velocity-dependence of frictional forces at sub 10 nm spatial resolution.

Figure a) and b) show experimental force quadrature curves for different probe heights. At low-amplitude (low-velocity) the tip is stuck and at higher amplitude (velocity) stick-slip behavior gives way to smooth sliding. Qualitatively similar behaviour is seen in the simulated force quadrature curves c) and d), derived from numerical integration of a modified Prandtl-Tomlinson model.



[1] arxiv:1601.07693

LUBRICANT FLOW IN AN ELASTOHYDRODYNAMIC CONTACT

Janet Wong

The Tribology Group, Department of Mechanical Engineering, Imperial College London, UK SW7 2AZ

Lubricants are frequently used to reduce friction and wear of machine components where moving parts are involved. In components such as rolling bearings, and gears, lubricants in tribological contacts is in the elastohydrodynamic (EHD) regime where lubricants experience a pressure typically greater than 1 GPa and the shear rate 10^5 - 10^7 s^{-1}. The thickness of EHD lubricant is commonly <1 μm. Hence how a lubricant behaves in ambient conditions and in EHD contacts can be very different. Understanding of rheology of EHD lubricant is crucial for friction prediction. While rheological models have been developed, there is no consensus on applicability of these models. This is mainly due to experimental difficulties in conducting *in-situ* measurements in EHD conducts. In this presentation, a summary on the commonly used rheological models for EHD lubricants will be given. Our recent effort in developing novel *in-situ* experimental techniques that allow information about rheological properties of lubricants in EHD contact to be obtained will be described. Interesting and in some cases, unexpected observations on EHD lubricants will be discussed.

MANIPULATION OF GOLD FUNCTIONALIZED NANOPARTICLES ON FLAT SUBSTRATES USING A HIGH FREQUENCY TRANSDUCER COUPLED TO AFM

Karine Mougin[1], Reinhold Wannemacher[2], Patricia Pedraz[2] and Enrico Gnecco[3]

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[2] IMDEA Nanociencia, C/Faraday, 9, Campus Universitario de Cantoblanco, 28049 Madrid, Spain
[3] Otto-Schott-Institut für Materialforschung, Löbdergraben 32, 07743 Jena, Germany

The mobility of gold nanoparticles (Au NPs) deposited on bare silicon wafers and controlled by AFM, is one of the few practical strategies for making ensembles of nanostructures. The mechanism that produces the organization of NPs is determined by the competing interactions between the components. The understanding and controlling of those interactions facilitate the realization of the fabrication of pre-designed nanostructures by this means.

In this work, Au NPs deposited on silicon substrates have been excited at high frequency using an out-of-plane transducer coupled with an AFM. Previous investigations have shown the absence of ultrasound-induced movement of NPs deposited onto silicon wafers or on SAW filters, for an in-plane and out-of-plane vibrations at MHz (Figure 1), as well as surface acoustic waves (of unknown polarization) due to strong adhesion of the particles to the substrates and relatively weak inertial forces caused by the ultrasonic vibrations.

The main objective of this work was to modulate the interactions between the substrate and the NPs by controlling their functionalization (hydrophobic and hydrophilic ones), and to manipulate these hundred of nm diameters Au NPs using a higher oscillation frequency to increase the acceleration of the Nps during manipulation. The NPs were manipulated in the frequency of the range of hundred of MHz.

Employing the well-known ultrasound-induced superlubricity [1], it is possible to image such particles without moving them and observe the effect of ultrasonic vibrations as a function of vibration amplitude and polarization. Alternatively, optical imaging in a conventional microscope could have been employed to localize particles of hundred of nm diameter without moving them in the case of sufficiently small coverage.

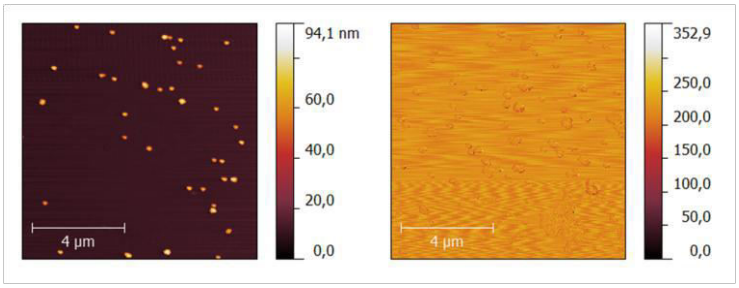

Figure 1 . Height images of citrate-coated gold NPs deposited onto a silicon wafer, a. before vibration, b. during application of in-plane vibrations of 2MHz.

[1] D. Kiracofe, A. Raman, D. Yablon “Multiple regimes of operation in bimodal AFM: understanding the energy of cantilever eigenmodes, Beilstein J. Nanotechnol., 4, 385–393(2013)

Poster session Tuesday, July 5, 16:20 – 18:40

1) Tarik Baytekin CONTROLLING FRICTION BY SURFACE TRIBOCHARGES

2) Andra Craciun INFLUENCE OF CTAB SURFACTANT ON GOLD NANORODS AFM-BASED MANIPULATION

3) Leonid Dorogin ELASTOHYDRODYNAMICS FOR SOFT SOLIDS WITH SURFACE ROUGHNESS: TRANSIENT EFFECTS

4) Annalisa Fasolino STATIC AND DYNAMIC FRICTION OF FRENKEL KONTOROVA MODELS IN TWO DIMENSIONS

5) Alkisti Gkouzou TEMPERATURE-DEPENDENT FRICTION BETWEEN LOCALLY HEATED MICROSCALE SURFACES

6) Evghenii Harea STUDY OF WEAR VARIATION DUE TO ENERGY DISSIPATION IN POLYPROPYLENE/RUBBER BLENDS

7) Benjamin Irving IN-SILICO DESIGN OF LAMELLAR MATERIALS FOR TRIBOLOGICAL APPLICATIONS

8) Evgeni Ivanov EFFECTS OF HARD AND SOFT NANOFILLERS ON FRICTION AND WEAR PROPERTIES OF POLYMER NANOCOMPOSITES

9) Davide Mandelli UNDERSTANDING FRICTION IN GRAPHENE / *h*BN HETEROJUNCTIONS

10) Nicola Manini DISSIPATION MECHANISMS IN SLIDING FRICTION

11) Diego Marchetto TESTING AND MODELING THE EFFECT OF ROUGHNESS ON FRICTION OF STEEL ON ICE

12) Pierre-Emmanuel Mazeran CALIBRATION OF LATERAL FORCE IN AFM USING THE EDGE METHOD AND A SCRATCH SAMPLE

13) Magnus Mets ELECTRON BEAM INDUCED SHAPE RESTORATION EFFECT IN Ag−SiO_2 CORE−SHELL NANOWIRES

14) Olivier Noel EXPLORING NANO-WEAR MECHANISMS OF CU-BASED COMPOSITES WITH THE AFM CIRCULAR MODE

15) Sven Oras MANIPULATION OF ZNO NANOWIRES BY PICK-AND-PLACE METHOD

16) Juozas Padrugskas NATURAL FRICTION MODIFIERS AND THEIR IMPACT ON FRICTION IN MACRO SCALE

17) Rémy Pawlak HYDROXYL INDUCED PARTIAL CHARGE STATES OF SINGLE PORPHYRINS ON TITANIA

18) Prashant Pendyala FRICTIONAL STUDIES ON HIERARCHICAL PATTERNS WITH VARIED SURFACE CHEMISTRY

19) Karina Pivnic MECHANISM OF ELECTROTUNABLE FRICTION MEASURED IN AFM EXPERIMENTS WITH IONIC LIQUIDS

20) Boris Polyakov 2D TRANSITION METAL DICHALCOGENIDES AS A SOLID LUBRICANT FOR NANOWIRES MANIPULATION

21) Rando Saar ELECTRON BEAM INDUCED GROWTH OF SILVER NANOWHISKERS

22) Hendrik Schmidt INFLUENCE OF THE NEAR SURFACE REGION ON FRICTION IN MANGANITES AND MULTILAYER FILMS

23) Borislav Vasic: GRAPHENE AS A PROTECTIVE COATING FOR MACROMOLECULES: AFM MANIPULATION STUDY

24) Borislav Vasic: WEAR PROPERTIES OF GRAPHENE STUDIED BY ATOMIC FORCE MICROSCOPY

25) Aleksandar Vencl DIFFERENCES BETWEEN MACRO- AND NANOHARNESS OF MMC MATERIALS

26) Sergei Vlassov TRIBOMECHANICAL CHARACTERIZATION OF INDIVIDUAL NANOSTRUCTURES SUPPORTED BY FEM SIMULATIONS

27) Dilek Yildiz ENERGY DISSIPATION MECHANISM ON LAYERED STRUCTURES

28) Zhenyu Zhang QUANTIFYING MINERAL SURFACE ENERGY BY SCANNING FORCE MICROSCOPY

CONTROLLING FRICTION BY SURFACE TRIBOCHARGES

H. Tarik Baytekin[1]

[1] Bilkent University-National Nanotechnology Research Center (UNAM), Ankara, Turkey,
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Tribo related events involve complex mechanisms that originate from the fact that both physical and chemical processes can take place at the same time during e.g. rubbing two polymer pieces to each other. Usually such physical treatments result in surface charging, known as tribocharging [1]. In this study, we aim to show that friction is highly affected by the generation of electrostatic (triboelectric) charges, which are produced on insulator surfaces as a result of mechanochemical changes on the surfaces. To verify this underestimated relation [2], tribocharges and coefficient of friction will be measured simultaneously using electrostatic voltmeter and a friction tester. As a complementary study, the occurrence of physical changes involving chemical changes, i.e. material transfer from a rubbed polymer to a metal or other polymer surface will be investigated to show the “heterogeneous” charge distribution of triboelectricity in friction. Then, charging and discharging the surfaces sequentially will help to control the friction. An externally applied ion source onto the tribocharged surfaces will be tried to control the friction (either increase or decrease) between the triboelectrified surfaces.

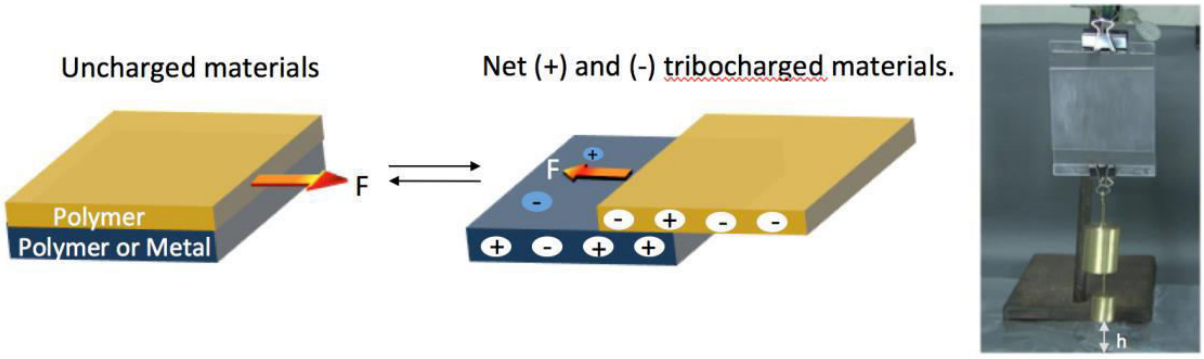

Figure 1. Tribocharging of insulators (left) and a weight can be lifted by tribocharged polymer sheets (right)

[1] H. T. Baytekin, A. Z. Patashinski, M. Branicki, B. Baytekin, S. Soh, B. A. Grzybowski. Science, 303, 308-312, (2011).

[2] T. A. L. Burgo, A. Erdemir, Angew. Chem. Int. Ed., 53, 12101-12105, (2014).

*HTB thanks to TUBITAK (project number 214M358) for supporting this research.

The Second European Workshop on Understanding and Controlling
Nano and Mesoscale Friction: July 4-7 2016, Riga, Latvia

INFLUENCE OF CTAB SURFACTANT ON GOLD NANORODS AFM-BASED MANIPULATION

A. D. Craciun, B. Donnio, J. L. Gallani and M. V. Rastei

Institut de Physique et Chimie des Matériaux de Strasbourg, CNRS, Université de Strasbourg, F-67034

We present an AFM-based nanomanipulation study of CTAB-functionalized gold nanorods on silica surfaces. Our findings reveal that the CTAB coating plays a key role in nanomanipulation process. AFM experiments on ordered CTAB films directly adsorbed on silica surfaces show that the layered molecules reduce both the friction and adhesion, as compared to pristine silica surface. By progressively increasing the molecular film thickness, up to several layers, we observe a non-linear variation of friction, with the lowest values in the low thickness regime. Our observations can be analyzed within asperity friction models which include local deformations of layered molecules. We have equally investigated the molecular organization of CTAB surfactant on different surfaces and its significance for friction and adhesion, thus obtaining useful guidelines for CTAB-functionalized gold nanorods manipulation on surfaces.

ELASTOHYDRODYNAMICS FOR SOFT SOLIDS WITH SURFACE ROUGHNESS: TRANSIENT EFFECTS

Leonid M. Dorogin[1], Michele Scaraggi[2,1] and Bo N. J. Persson[1,3]

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[3] www.MultiscaleConsulting.com

A huge number of technological and biological systems involves the lubricated contact between rough surfaces of soft solids in relative accelerated motion. Examples include dynamical rubber seals and the human joints.

In this study we consider an elastic cylinder in accelerated sliding motion on a rigid, randomly rough substrate in a fluid. We calculate the surface deformations, interfacial separation and the contributions to the friction force and the normal force from the area of real contact and from the fluid. The driving velocity profile as a function of time is assumes to be either a sine function, or a linear multi-ramp function. We also calculate the steady state friction coefficient as a function of sliding speed (the Stribeck curve, see [1]).

In all cases we assume the surface roughness to be self-affine fractal and the fluid is treated as a Newtonian fluid i.e. the fluid viscosity is assumed independent of the shear rate. Simulation of real experimental conditions of accelerated sliding is also performed and compared with the experimental data.

[1] B. N. J. Persson and M. Scaraggi // Lubricated sliding dynamics: Flow factors and Stribeck curve, Eur. Phys. J. E (2011) 34: 113, DOI 10.1140/epje/i2011-11113-9.

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STATIC AND DYNAMIC FRICTION OF FRENKEL KONTOROVA MODELS IN TWO DIMENSIONS

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[1] Department of Physics, Stockholm University, 106 91 Stockholm, Sweden
[2] Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen,
[3] Department of Engineering Design and Materials, Norwegian University of Science and Technology, Trondheim, NorwayInstitution

The Frenkel Kontorova (FK) model in one dimension (1D) is a simple model that provides a base for the understanding of sliding friction. Extensions to 2D would be useful to describe real interfaces but the choice of model and parameters controlling the coupling of dynamics in the two directions is not trivial. We study the two most straightforward extensions of the FK model to two dimensions and simulate both the static and dynamic properties. The behavior of the static friction is similar in 1D and 2D. The dynamic friction, however, is strongly influenced by the second dimension and the accompanying additional dynamics and parameters introduced into the models. Following ref.1. we discuss our results in terms of the thermal equilibration and phonon dispersion relations of the lattices, establishing a physically realistic and suitable two-dimensional extension of the FK model. The presence of additional dissipation channels can increase the friction and produces significantly different temperature-dependence when compared to the one-dimensional case. We show that the anisotropy of the dynamic friction leads to new effects, including that the direction of the motion can depend on the magnitude of the velocity [2].

[1] J. A. van den Ende, A. S. de Wijn, and A. Fasolino. The effect of temperature and velocity on superlubricity. J. Phys. Cond. Mat., 24:445009, 2012

[2] J. Norell, A.Fasolino and A. S. de Wijn Emergent friction in two-dimensional Frenkel-Kontorowa models, arxiv 2016

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TEMPERATURE-DEPENDENT FRICTION BETWEEN LOCALLY HEATED MICROSCALE SURFACES

Alkisti Gkouzou[1], Jaap Kokorian[1], Guido C. A. M. Janssen[1], W. Merlijn van Spengen[1,2]

[1] Delft University of Technology, Mekelweg 2, 2628 CD Delft, The Netherlands

[2] Falco Systems BV, Van Boshuizenstraat 12, 1083 BA Amsterdam, The Netherlands

In this work, we investigate how capillary condensation affects friction between two sliding surfaces in micro-electromechanical systems (MEMS) at different temperatures. AFM studies, which examined the nucleation of a capillary meniscus between a sliding tip and a substrate, demonstrated that water, in combination with contaminants, increases friction [1, 2].

Friction at the nanoscale is commonly studied with an AFM. Present-day models describe satisfactorily how energy is dissipated during sliding, assuming single-asperity contact between an atomically sharp tip and a substrate. However, these models cannot explain observed phenomena in MEMS devices due to the multi-asperity nature of two contacting microscale surfaces. For this study, we use a polycrystalline silicon-based MEMS tribometer that consists of a 'ram' and a sliding counter-surface, both connected to comb-drive actuators (Figure 1). The counter-surface can be heated *in situ* by Joule heating. We detect the motion of the counter-surface with sub-nm and sub-nN resolution using an optical displacement measurement technique based on curve-fitting [3]. We capture the undisturbed motion, and we can also observe the stick-slip motion of the counter-surface while it is in contact with the ram. The difference between the two motions, multiplied by the stiffness of the counter-surface's support springs, gives us the friction force.

The relationship between the temperature of the counter-surface and the applied heater power is calibrated using micro-Raman spectroscopy. We measured both the undisturbed and the stick-slip motion of the counter-surface at a constant normal force of 280 nN, at increasing temperatures ranging from 25 °C to 300 °C. We also measured the stick-slip motion for the same device at temperatures of the counter-surface decreasing from 300 °C to 25 °C. At higher temperatures, where there is no water at the contact, friction increases. Below 100 °C, the mixture of water and contaminants lubricates the contact, which reduces the dissipated energy (Figure 2).

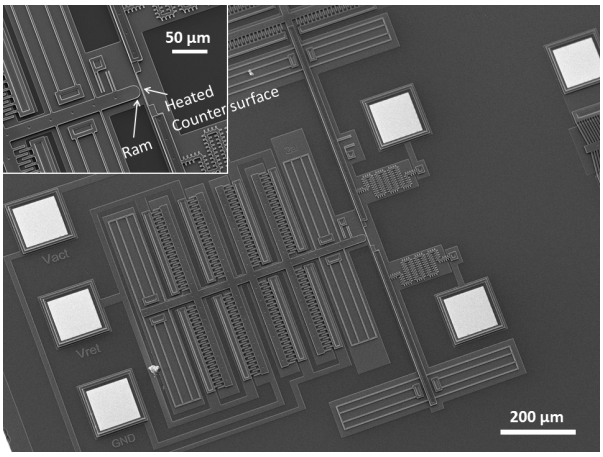

Figure 1: A MEMS tribometer with a heated counter-surface.

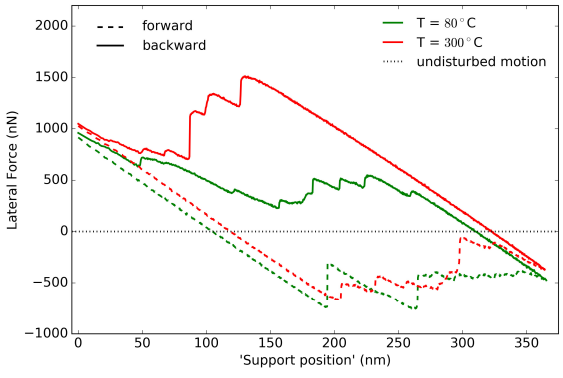

Figure 2: Friction in MEMS at 80 °C and 300 °C, plotted as 'AFM-like' friction loops.

[1] Jinesh K B and Frenken J W M 2006 *Phys. Rev. Lett.* **96** 166103
[2] Greiner C, Felts J R, Dai Z, King W P and Carpick R W 2012 *ACS Nano* **6** 4305–4313
[3] Kokorian K, Buja F and van Spengen W M 2015 *J. Microelectromech. Syst.* **24** 618–625

STUDY OF WEAR VARIATION DUE TO ENERGY DISSIPATION IN POLYPROPYLENE/RUBBER BLENDS

Evghenii Harea[1, 2]

[1] Institute of Applied Physics, Moldova,
[2] Tomas Bata University, CPS, Czech Republic.

Thermoplastic elastomers (TPEs) are generally a combination of thermoplastics and elastomers. They exhibit properties of elastomers but can be processed like thermoplastics. The most important feature of TPEs is recyclability of scrap and rejects in manufacturing process as well as of used TPEs products [1]. On the other hand, easy recycling and repairing is the factor that emphasis the use of thermoplastic elastomers over conventional thermoset rubbers.

The main goal of this study was investigation of variation of the friction coefficient and wear in the cycling friction test (ball-on-flat) for different holding time between the passes. The materials to be investigated are: Polypropylene (PP) blended with: (1) natural rubber (NR), (2) styrene-butadiene rubber (SBR), and (3) a mixture of 50%SBR+50%NR.

The well-known fact is the variation of mechanical properties of polypropylene (PP) based blends due to the testing speed during the tensile test. These phenomena are explained by the polymer chains alignment during the tensile test [2]. For the low speed tests, the energy dissipation enables more regular arrangement of the polymer chains and increases the quantity of such molecules.

The ball-on-plate tests were performed on a micro-friction machine (UMT-3 Bruker company) offering friction evaluation and wear testing facilities. Wear tests were carried out in air at room temperature using a stainless still ball of 2 mm diameter sliding against TPRs materials. Experiments show a considerable increasing (up to 50%) of the wear due to holding time after ball pass in ball-on-plate reciprocal test as well as friction coefficient variation. SEM images show the PP matrix orientation caused by friction and energy dissipation during this process.

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IN-SILICO DESIGN OF LAMELLAR MATERIALS FOR TRIBOLOGICAL APPLICATIONS

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Materials that exhibit *superlubricity* – whereby the frictional force is less than the lower-end detection limits achievable in macroscopic measurements [1] - are becoming increasingly important in engineering applications, as manufacturers look to reduce friction and wear of machine components. Friction is a retarding force that continually opposes the desired action of mechanical components; for example, upwards of 20% of automotive engine power may be spent in overcoming frictional resistance of moving parts. In order to reduce friction between surfaces in mutual contact, we must reduce the adhesive forces that exist between the microscopically irregular contact regions, *i.e.* surface asperities. This is typically achieved by introducing an oil-based lubricant to the interface between the layers. Although synthetic wet lubricants are continually improved, extreme operating conditions (think aerospace applications) can render them useless. In order to circumvent any potential shortcomings, *dry lubricants* such as molybdenum disulfide, MoS_2, and other members of the transition metal dichalcogenide (TMD) family of materials have come to the fore. Owing to their lamellar structures, TMDs (most commonly MoS_2) are suitable for use in tribological fields, yet little is known about the atomistic interactions occurring at the interface of the MX_2 layers. *Via* calculations performed within the density functional theory, we have performed a rapid assessment of the intrinsic frictional properties [2] of lamellar materials, improving our understanding of (bi)layer stability and tribological behavior: phenomena that are dependent on the interplay between electrostatics and van der Waals forces [3]. We not only elucidate the mechanism(s) underlying tribological phenomena, but we can also guide the design and fabrication of ultralow friction devices *via* new computational workflows. Moreover, in terms of expanding the range of properties achievable by TMD-based materials, we consider doped and alloyed species [4-5] as well as TMD/TMD *heterostructures*[6]. Their hybridization produces materials of novel functional composition, with the aim of tuning their chemical, physical and electronic properties for optimum performance.

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[4] H.-P. Komsa et al, Phys. Rev. B, 2013, 88, 035301

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EFFECTS OF HARD AND SOFT NANOFILLERS ON FRICTION AND WEAR PROPERTIES OF POLYMER NANOCOMPOSITES

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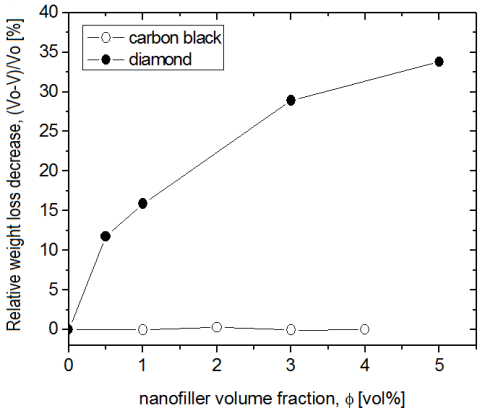
The advantages of nano-reinforcement over traditional filling materials open new frontiers of polymer nanocomposites in an ever growing range of applications, including surface protection [1,2]. The present study is concentrated on improving of surface properties (hardness, wear resistance, scratch and friction) of bulk polymers and coatings by nano-reinforcement with nanodiamond, multiwall carbon nanotubes and carbon ash. The aim is to study the effect of hard and soft nanofiller on the reinforcement and the surface properties of two types of polymer matrices (a thermoset and a thermoplastic polymer). The incorporation of small amount of hard and soft carbon nanofillers, such as nanoscale diamond, carbon ash and multiwall carbon nanotubes (MWCNT) have different effect on the surface properties of the neat polyester resin and polypropylene.

The addition of a small amount of nanofiller diamond (0.5–5%) as a nanofiller in polyester matrix leads to improving by more than 35% wear resistance of the polyester resin. The addition of hard nanofiller, such as diamond, contributes to a significant enhancement of the hardness of polyester resin nanocomposites. On the other hand, polyester matrix containing soft nanofiller – graphite/diamond ash (carbon black), has no an impact on the wear properties of the polyester resin.



Relative weight loss Decrease (Vo-V)/Vo (%) vs. volume concentration of diamond (full circles) and graphite/diamond (empty circles) in a polyester resin

MWCNT/iPP (polypropylene) composites containing low nanotube rate of 0.1 wt% results in a sharp decrease of the scratch depth, while further increase of the MWCNT content, from 0.1% to 3 wt%, results in a linear decrease of this characteristic. The friction coefficient is strongly improved by increasing the nanotube content. The 3 wt% MWCNT content produces significant improvement (47, 53 and 36%, respectively) of the three characteristics (hardness, scratch and friction coefficient) if compared to those of the neat iPP. The mechanical percolation of polypropylene containing MWCNTs appears at much lower nanotube content (2 wt%) compare with the polyester/diamond nanocomposites (4 vol%). On the other hand, it was found that the addition of second soft nanofiller (organoclay) to the PP matrix does not influence the coefficient of friction at scratch.

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UNDERSTANDING FRICTION IN GRAPHENE / *H*BN HETEROJUNCTIONS

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Relevant for applications in nano- and micro-motive components is the search for robust incommensurate superlubric interfaces. At the moment heterojunctions of rigid layered materials seem to be the best choice for such applications [1-2] with graphene and boron-nitride as promising candidates since they provide both adequate robustness and incommensurability. A detailed theoretical description of such system is therefore mandatory as it will serve as a solid background for the interpretation and the design of future experiments.

We present results of numerical simulations of the static and dynamical properties of hBNgraphene heterojunctions, performed adopting a recently developed inter-layer potential for Graphene/h-BN heterostructures [3]. In order to understand the relevant features determining the frictional response of the interface, we investigate the effects caused by variation of the interface relative angular misalignment, the external load and the size of the slider. In particular we focused on the role played by the periodic out-of-plane distortions which characterize the Moiré pattern of graphene layers adsorbed over incommensurate substrates [4-5]

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The Second European Workshop on Understanding and Controlling
Nano and Mesoscale Friction: July 4-7 2016, Riga, Latvia

DISSIPATION MECHANISMS IN SLIDING FRICTION

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A point slider grazing a flat crystalline surface represents the simplest contact where energy dissipation - friction - occurs.

We simulate the 1D and 2D model description of this contact.

This investigation reveals a highly nontrivial dependence of friction on the sliding speed, with generally extremely low friction at supersonic speed, larger friction at speeds comparable to the speed of sound, and multiple dissipation peaks at speeds of the order of 10% of the speed of sound.

The 1D model is so simple that an analytic treatment is possible in the weak-coupling limit.

In 2D we evaluate the separate frictional contribution of the vertical (transverse) displacements of the slider induced by the atomic surface corrugation.

TESTING AND MODELING THE EFFECT OF ROUGHNESS ON FRICTION OF STEEL ON ICE

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Due to the challenging fundamentals aspects and importance in a wide-range of fields, the study of friction between metals and ice is still actual even after decades of research. The mechanism of sliding on ice is mainly related to the existence of a layer of water on the ice surface itself. The thickness of this layer defines the working regime of the sliding system [1] and it is affected by the temperature of the environment, the normal force applied by the slider and the sliding velocity. Varying the experimental parameters it is possible to change the water layer thickness and to move through all lubrication regimes, from boundary to hydrodynamic. The analysis of the friction of ice is also complicated by the changing impact of the surface morphology of the slider at different lubrication regimes on ice.

This work studies the transition between different friction regimes and the role of the surface of the slider in terms of roughness, topography and wettability. We examined a “stainless steel-ice” contact as case study. Tribological tests were performed varying separately temperature and sliding velocity. We studied the dependence of friction from surface morphology by inducing different degrees of roughness on stainless-steel surfaces. Stainless steel was chosen as material for the slider because it is a good thermal conductor. In order to investigate the role of frictional heat we repeated the pin-on-disc tests using a slider made of an epoxy resin with a thermal conductivity about 100 times lower than that of steel.

Parallel to the experimental work we developed an analytical model (based on the one of Makkonen [2]) to explain the correlation between the surface roughness of the slider, the lubrication regime (related to the water layer thickness) and the measured friction coefficient. The model takes into account the solid contact between two sliding asperities and describes the local CoF between them in terms of shear stress of the LLL originated from the melting of ice at the interface.

Authors would like to acknowledge the support from COST ACTION MP1303.

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CALIBRATION OF LATERAL FORCE IN AFM USING THE EDGE METHOD AND A SCRATCH SAMPLE

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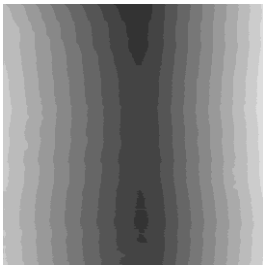
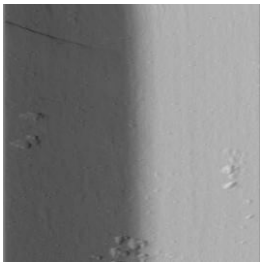
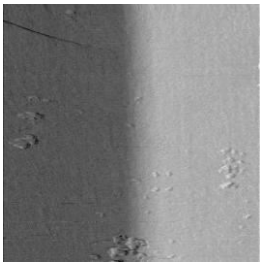
The edge method [1] is one of the most popular methods to calibrate lateral force in AFM experiments. It is based on the fact that the LFM signal is both sensitive to the friction force and the slope of the sample α in the scanning direction. These two components could be separated by making the difference (T-R) and the sum (T+R) of the trace and the retrace LFM images: The two images are respectively a friction and a slope images and could be used for calibration. Theoretically, any sample that presents variation of slope and constant friction coefficient could be used for calibration. Practically, the ideal sample for calibration is not so easy to be found: The sample should have huge domains with constant slope and friction coefficient in the scanning direction to be able to connect the variation of the slope to the variation of the LFM signal. We propose to use a fused silica sample that has been scratched by a Berkovich tip of a nanoindenter (Fig. a). AFM images show that the scratch presents two different constant slopes (Fig. b), and a constant friction coefficient by means of the T-R image (Fig. d). Thus, the sample could be considered as homogeneous and the T+R image (Fig. c) should be proportional to the product of the slope by the load. Both the slope and the T+R images present two Gaussian populations that correspond to the two sides of the scratch (Fig. e & f). The ratio of the difference between the average values of these two populations (ΔLFM/Δα) gives directly the calibration factor if the load is known. By repeating imaging with different loads, the ratio of ΔLFM/Δα is found to be proportional to the load and the calibration factor could be easily calculated (Fig. g).



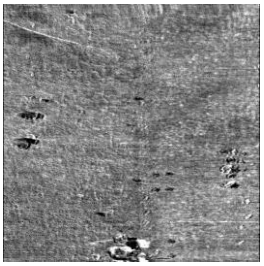
(a) ΔZ=221nm



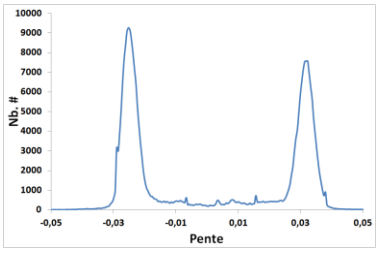
(b) ΔZ=0.16



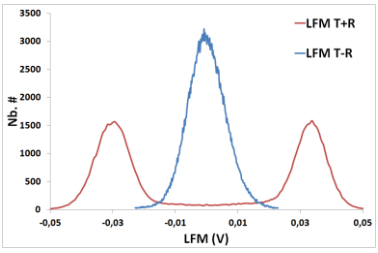
(c) ΔZ=0.19V



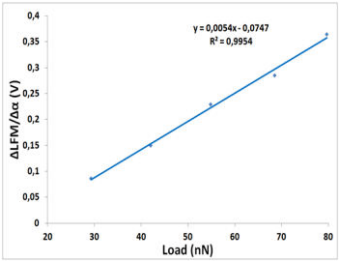
(d) ΔZ=0.046V



(e)



(f)



(g)

Topo (a), slope (b), LFM T+R (c) and LFM T-R (d) images of the scratch. Histograms of slope (e) LFM T+R and T-R (f). ΔLFM/Δα as a function of the load (g), slope gives the calibration factor.

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ELECTRON BEAM INDUCED SHAPE RESTORATION EFFECT IN AG−SiO_2 CORE−SHELL NANOWIRES

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In present work we investigated mechanical properties of Ag−SiO_2 core−shell NWs produced by coating chemically synthesised silver NWs with SiO_2 shells according to a well-established sol−gel chemistry method.

We performed half-suspended beam-bending tests on Ag−SiO_2 core−shell nanowires inside a scanning electron microscope (figure 1) and demonstrated enhanced fracture resistance and electron beam promoted shape restoration effects [1]. Shape restoration was shown to be a phenomenon exclusively inherent to core−s hell heterostructures, and absent for pure Ag NWs or SiO_2 shells separately. Shape restoration was explained as e-beam induced structural relaxation of the SiO_2 shell governed by elastic forces generated by the deformed Ag core.

Test conditions were simulated using FEM, and the average value of e-beam induced viscosity of the shell $\eta = 7 \times 10^{11}$ Pa.s was extracted by fitting simulated relaxation curves with experimental data. The stresses in the core of core−shell NWs in bending experiments can reach to 15 GPa without visible fracture, in contrast to uncoated Ag NWs, which start to fracture at a stress of 8.5 GPa. According to finite element method simulations, the shell can dampen the mechanical stresses in the core in the vicinity of the contact with a stiff substrate and mitigate the plastic yield in the core. To the best of our knowledge, this is the first experimental work on the mechanical characterization of metaloxide core−shell Nws.

The reported results clearly demonstrate that the combination of two different materials in a single composite core−shell heterostructure can lead to improved or even completely novel properties.

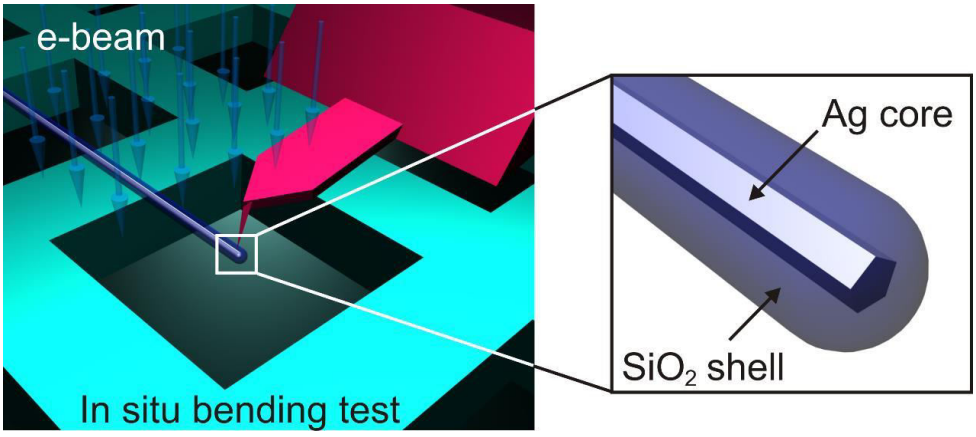

Figure 1. Schematics of the bending test inside scanning electron microscope

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EXPLORING NANO-WEAR MECHANISMS OF CU-BASED COMPOSITES WITH THE AFM CIRCULAR MODE

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Wear tests were performed using the AFM circular mode [1], in dry condition, on two Cu-based composites reinforced with added micro-sized (approx. 750 nm) and in-situ generated nano-sized (< 100 nm) Al_2O_3 particles. The nano-sized material shows a well lower wear rate (1/500) at the macroscale [2]. The circular mode allows measuring wear rate at the nano-scale (i.e. in the matrix) in stationary conditions with high sliding velocities (up to 1 mm/s) by obtaining well defined circular wear tracks. Topographic images of the various wear tracks have been measured to determine the wear rate for different parameters such as the sliding speed, the normal force and time. Results show that the nanosized composite has, also at the matrix level, a well lower wear rate suggesting that the decrease of the macroscopic wear rate is also due to a modification of the wear matrix behaviour (figure 1). The different behaviours of the wear rate with the different experimental parameters will be also shown and discussed in terms of wear mechanisms.

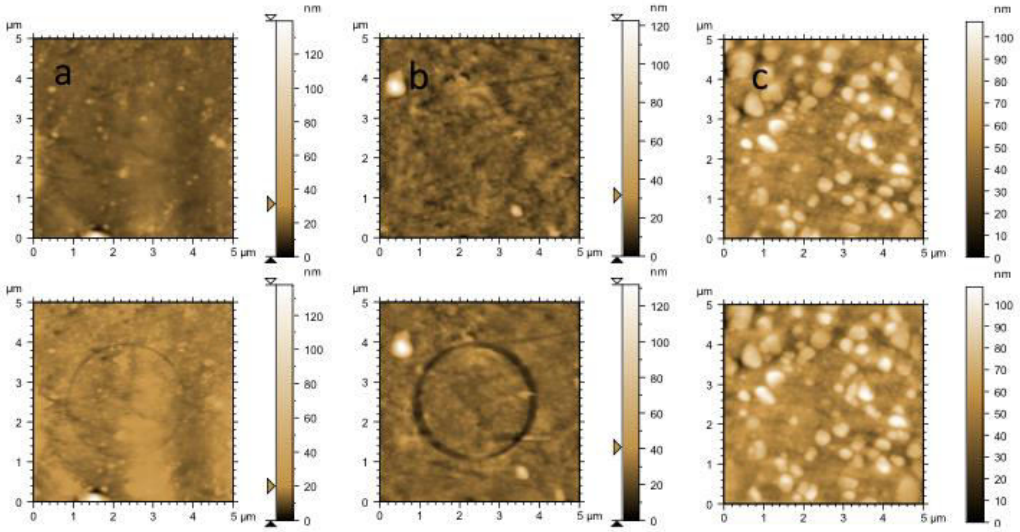

Figure 1: Topographic images of wear tracks on Cu-based composite charged with (a) and (b) micro-alumina Al_2O_3 and (c) nano-Al_2O_3-alumina particles using the AFM circular mode: Before (Top) and after (bottom) wear experiments.

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MANIPULATION OF ZNO NANOWIRES BY PICK-AND-PLACE METHOD

Sven Oras[1], Boris Polyakov[2], Mikk Vahtrus[1], Mikk Antsov[1], Andris Šutka[1,3], Leonid Dorogin[1,4], Andres Juur[1] , Rando Saar[1], Rünno Lõhmus[1] and Sergei Vlassov[1]

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ZnO nanowires (NW) are attractive objects for performing tribology experiments. Their hexagonal cross-section and well defined facets [1] enable us to easily approximate contact areas during experiments while the elastic properties [2] of the NWs makes it possible to measure friction forces from their profile without using an external force sensor. In these experiments NWs were manipulated into a suitable location using the “pick and place” approach. Static and kinetic friction was measured. Median value of the maximal interfacial shear strength of the contact calculated in 16 bending tests was found to be 1.3 ± 0.7 GPa. The friction force values for kinetic friction measurements were highly scattered being mostly below 15 MPa.

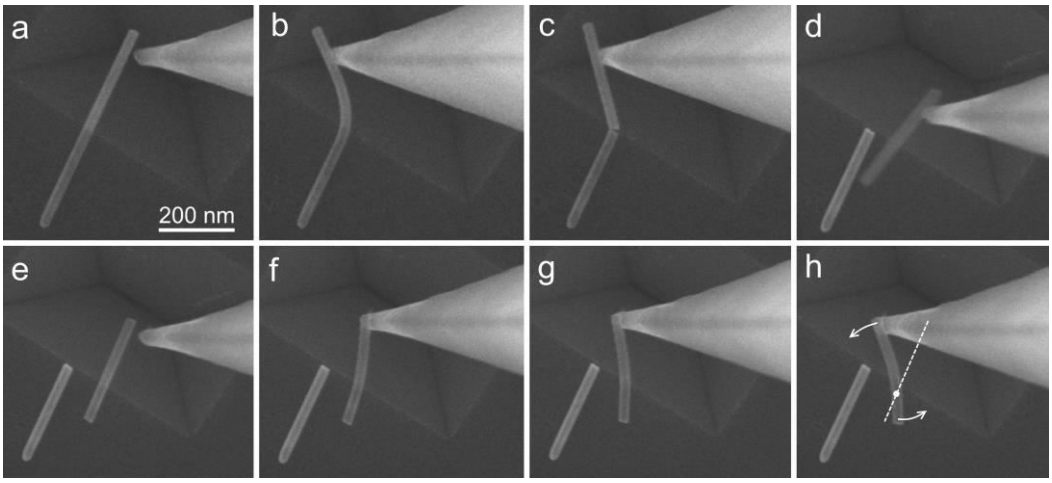

Figure 1.Typical manipulation of half-suspended ZnO NW inside HRSEM: (a-c) bending and breaking of the NW, (d-e) pick-and-place manipulation, (f-g) static friction measurements, (g-h) bent NW is rotating.

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[2] L. M. Dorogin, Phys. Status Solidi (b) 250, 35 (2013)

NATURAL FRICTION MODIFIERS AND THEIR IMPACT ON FRICTION IN MACRO SCALE

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Aleksandras Stulginskis University, Lithuania

Adsorption of oil molecules on the surface has a large influence on lubrication properties. Fatty acids are one of the naturally appearing friction modifiers which are very effective in reducing friction [1].Their absorption properties in various solutions have been broadly investigated. It was found that the absorption of fatty acids on the lubricated surfaces, and their strength is determined by its nature [2], concentration [3], loads and surface interaction speeds [4], and temperature [5]. Saturated and unsaturated fatty acid molecules, with different electronic structure, differently adsorb on metal surface.

All the conditions as well as strength of adsorbed layer vary during friction process. Increasing the temperature changes the adsorption layer and the metallic surface energy balance, thus reducing its strength. The layer also can be removed by surface mechanical interaction. No less important is how fast can recover damaged adsorption layer.

Nano-, micro- and macro scale investigation results not always coincides, so it is difficult to predict how the adsorbed layer will behave under certain conditions.

In this study we investigated the influence of temperature and contact pressure on friction properties of naturally appearing friction modifiers. Test were performed on pin-on-disc tribometer, using bearing steel friction elements lubricated with vegetable oil having mostly mono unsaturated fatty acid structure. It was observed that in certain temperature sharp drop in friction occurs. The process seems to be resetting.

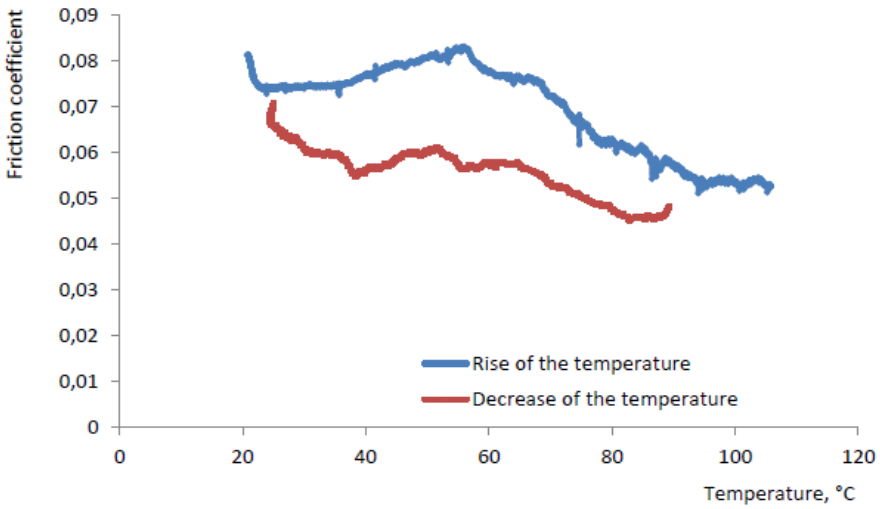

Fig. 1 Temperature influenced variation of friction coefficient

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HYDROXYL INDUCED PARTIAL CHARGE STATES OF SINGLE PORPHYRINS ON TITANIA

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The adsorption of Cu-porphyrin derivatives terminated with peripheral carboxyphenyl side groups on hydroxylated TiO_2(110) surfaces is investigated by combined scanning tunneling microscopy (STM), atomic force microscopy (AFM) and density functional theory (DFT). Two distinct contrasts of the molecules are revealed by STM and tunnelling spectroscopy. Via controlled manipulations of single molecules, the origin of these peculiar contrasts is found to arise from the presence or not of hydroxyl groups below the molecules. Hence, the electronic coupling of the molecule with the underlying TiO_2 surface is locally modified altering the amount of charge transfer and thus their charge state at the molecular scale. Our results particularly underline the fundamental role of hydroxyls of TiO_2 on the charge state of adsorbed organic molecules potentially used in dyesensitized solar cells.

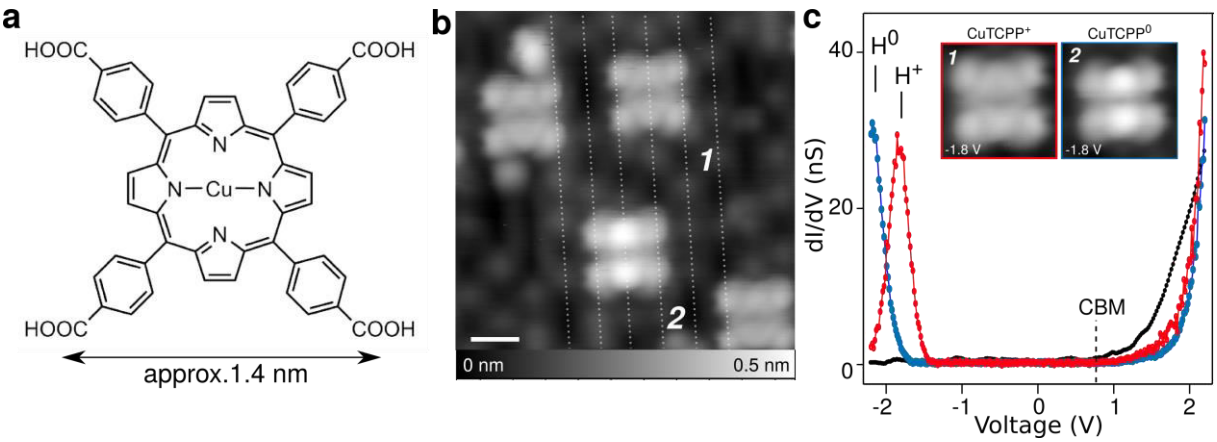

Figure 1: (a) Molecular structure of the porphyrin derivative equipped with carboxyphenyl end-groups. (b) STM image of the two porphyrin contrasts on TiO_2(110) (b) Conductance spectroscopy of the two molecular configurations suggesting a modulation of their charge state

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FRICTIONAL STUDIES ON HIERARCHICAL PATTERNS WITH VARIED SURFACE CHEMISTRY

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Hierarchical patterns are expected to reduce the frictional characteristics of surfaces. However individual role of micro and nano scale geometrical features in the overall performance of the surfaces is not yet understood completely. Especially the effect of geometry and pitch of the nanoscale features is not explore significantly in part due to the complexity involved in the fabrication of such structures. We study the frictional characteristics of 2-level hierarchical surfaces in Si and PMMA generated using capillary force lithography technique. The surface chemistry of the patterns is varied using DLC, Z-dol on Si surfaces and using PTFE on PMMA surfaces. Frictional behavior of the surfaces was investigated using AFM at different relative humidity levels (5% to 80%) and applied normal loads (40 nN to 120 nN). We show that increase in pitch of the nanoscale features significantly influences the frictional resistance of the patterned surface. The effective role of the microscale features of the hierarchical patterns is observed to be in decreasing the effective interaction volume and thereby the magnitude of resistive forces. It is observed that capillary forces originating from the condensed water vapor in the narrow gaps between indenter and nano scale features play a crucial role in the overall tribological performance. A correlation between frictional force and real/projected area brought the multi asperity interaction behavior in contrast to the single asperity contact condition predicted by the contact mechanics models.

Figure 1: Schematic of a spherical indenter sliding on a 2-level hierarchical pillar patterned surface

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MECHANISM OF ELECTROTUNABLE FRICTION MEASURED IN AFM EXPERIMENTS WITH IONIC LIQUIDS

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The interest in the molecular mechanisms of layering and friction of ionic liquids (IL) in electrified nanometer confinements has led to experimental force sensitive measurements employing atomic force microscope (AFM) [1-4]. Super-low friction (superlubricity) was demonstrated [3-4] to be switched on and off in situ, by polarizing the surface relative to the reference electrode, switching either to anion enriched or cation enriched layer. Using molecular dynamics simulations, we simulate a system mimicking such experiments. We focus on understanding a mechanism of electrotunable friction measured in AFM experiments when only one layer of IL is present between the surfaces. In particular, we investigate how does the orientation of the interfacial cation layer influences the friction and adhesion at such tribological contacts.

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2D TRANSITION METAL DICHALCOGENIDES AS A SOLID LUBRICANT FOR NANOWIRES MANIPULATION

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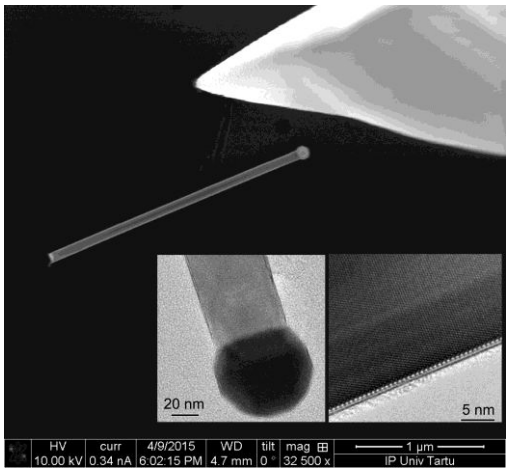
Highly oriented pyrolytic graphite and graphene are known to be low friction materials, and numerous nanomanipulation experiments were performed on these substrates [1]. Layered transition metal dichalcogenides (TMDs) such as WS_2 and MoS_2 have attracted recently an increasing attention due to ease of their synthesis and number of beneficial properties [2]. These TMDs are extremely chemically inert and non-toxic, widely used as a lubricant additive [3]. In this work we synthesized WS_2 and MoS_2 2D crystals on silicon wafer as substrates for ZnO nanowires and core-shell ZnO-WS_2 nanowires manipulation. The experiments were performed inside a scanning electron microscope (SEM) equipped with a nanomanipulator with an atomic force microscope (AFM) tip as a probe. Nws were pushed by the tip from one end until complete displacement is achieved, while NW bending is monitored by the SEM. The elastic bending profile of a NW during the manipulation process is used to calculate the static and kinetic friction forces by method described in our previous work [4].



SEM image of ZnO-WS_2 nanowire on silicon wafer in proximity of AFM tip (inset: TEM images).

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ELECTRON BEAM INDUCED GROWTH OF SILVER NANOWHISKERS

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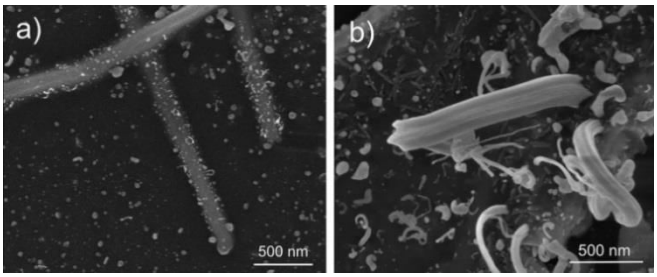
In this work we report an electron beam induced rapid (up to several tens of nm/s) growth of silver nanowhiskers from silver nanowire networks coated with TiO_2 by sol–gel method. Different growth conditions are tested and it is demonstrated that growth is optimal for samples with the film thickness in the range 50–200 nm and previously annealed at 400 °C for 5–10 min. The SEM characterization showed that the diameter of the Ag whiskers varies from few nm to several hundred nm, the growth rate was up to several tens of nm/s and the whiskers may grow from a few nm to several micrometres in length before the growth terminates. No considerable dependence of whiskers growth on electron beam parameters (voltage and current) was established. Growth mechanism is attributed to cooperative effect of several factors including diffusion of Ag into TiO_2 matrix during annealing, electromigration of Ag atoms caused by strong electric field, and presence of mechanical stresses at interfaces enhanced by thermal expansions due to local heating under e-beam illumination.



Electron beam induced growth of Ag whiskers from the TiO2 coated AgNWs network annealed at 400ºC for 30 min.

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INFLUENCE OF THE NEAR SURFACE REGION ON FRICTION IN MANGANITES AND MULTILAYER FILMS

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We investigate how the electronic properties of a material affect its surface friction. Specifically we use lateral force AFM to measure the friction of manganite thin films that can be switched between a conducting and insulating state. These materials provide an ideal way to systematically vary material properties by external control parameters without changing the topology or chemistry of the sample surface.

Recent literature studies [1-3] report a clear change in measured friction when the electronic state of the material is altered. We investigate the friction of a manganite film ($La_{0.55}Ca_{0.45}MnO_3$) for which the electrical resistance can be reversibly varied over several orders of magnitude by changing the temperature or by resistive switching. In contrast to the results presented in literature [1-3], we have not yet observed a change in friction that can be attributed to the temperature-induced metal-insulator transition. However, we do see a reproducible and significant reduction in friction if we resistively switch a local region of the manganite film using sufficiently high voltages [4] from the insulating to the conducting state. Possible explanations for these apparently contradictory observations will be discussed on the poster.

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[4] J.-O. Krisponeit et al., Phys. Rev. B 82, 144440 (2010)

GRAPHENE AS A PROTECTIVE COATING FOR MACROMOLECULES: AFM MANIPULATION STUDY

Borislav Vasić[1], Aleksandar Matković[1], Jelena Pešić[1], Julia Prinz[2], Ilko Bald[2,3], Aleksandar Milosavljević[1], and Radoš Gajić[1]

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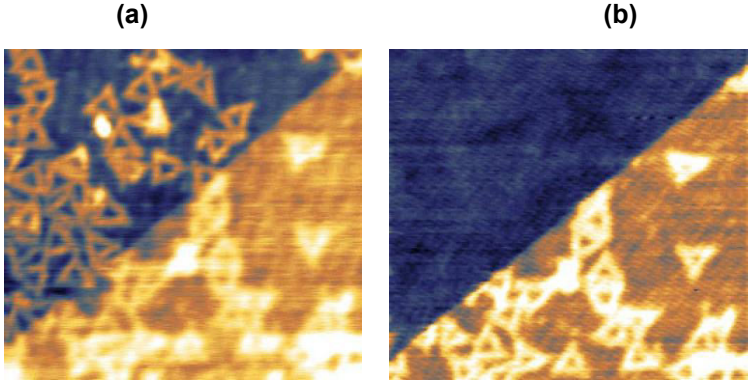
Graphene is an ultrathin material with excellent mechanical properties. Therefore, it can be used for various very compact protective coatings, mostly for friction and wear reduction. At the same time, graphene is flexible, so it can easily cover nanoparticles and molecules following their shape. Here we study graphene efficiency as a protective coating for macromolecules such as DNA origami structures [1]. For this study, we use atomic force microscopy (AFM) based manipulation in the contact mode. We show that graphene enables imaging of triangular DNA origami structures at one order of magnitude higher normal load compared to the case of bare and unprotected molecules.



(a) Topography recorded in the tapping mode before AFM manipulation. Triangular DNA oriami structures are visible both on bare silicon-dioxide substrate (blue area) as well as below graphene (yellow area). (b) Topography recorded in the contact mode during the AFM manipulation. DNA origami structures are still visible below graphene and they are undamaged. On the other hand, bare DNA origami structures are completely removed on silicon-dioxide. Scan size in both images is 1x1 μm^2

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WEAR PROPERTIES OF GRAPHENE STUDIED BY ATOMIC FORCE MICROSCOPY

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Applicability of graphene for protective coatings mostly depends on its wear resistivity. In order to study wear properties on nanoscale, we use scratching technique based on atomic force microscopy (AFM) in the contact mode. We consider both chemical vapor deposition (CVD) graphene as well as exfoliated graphene. It is shown that wrinkles in CVD graphene significantly decrease its wear resistivity [1]. Wrinkles are out of plane deformations of graphene, so the contact area between AFM tip and them is increased leading finally to enhanced lateral forces and graphene tearing for lower normal loads. In the case of exfoliated graphene, it is shown that graphene edges are onset of wear. AFM probe going across graphene edge leads to elastic strain at low normal loads, then to wrinkle formation and plastic deformation at intermediate loads, and finally to graphene tearing at high normal loads.

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DIFFERENCES BETWEEN MACRO- AND NANOHARNESS OF MMC MATERIALS

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Metal matrix composite (MMC) materials are very inhomogeneous materials and their properties depend on various parameters (production process, constituents and their interfaces, etc). Macro-, micro- and nanohardness of the same material can be very different, depending on the position of indentation. Four hybrid A356/SiC_p/Gr_p composites were tested. They were produced by compocasting process using Al-Si alloy matrix (A356), silicon carbide (SiC_p) microparticles (40 μm) and graphite (Gr_p) macroparticles (200-800 μm), with additional T6 heat treatment (Fig. 1a). The amount of incorporated silicon carbide was 10 wt. %, while the amount of graphite was 1, 3 and 5 wt. % [1]. Macro hardness measurements were performed using the Vickers hardness tester with 5 kg load. Nanohardness measurements were performed using the nanoindenter with Berkovich indenter and maximum load of 5 mN (Figs. 1b and 1c). Locations of the measurement were different (Table 1). There is no correlation between macro- and nanohardness. Nanohardness measurement allowed characterization of distinct regions and analysis of the influences of single composite constituents.

Acknowledgement: This work has been performed as a part of activities within the project TR 35021 supported by the Republic of Serbia, Ministry of Education, Science and Technological Development, whose financial help is gratefully acknowledged.

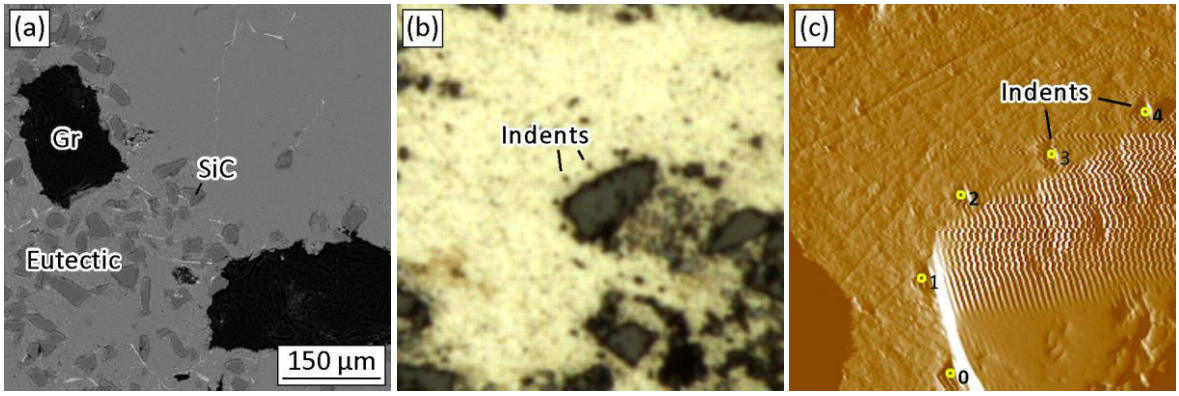

Figure 1: Hybrid composite: (a) microstructure (SEM image), (b) nanoindents (OM image) and (c) nanoindents (SPM image 40 x 40 μm)

Composite designation	Macrohardness HV5	Nanohardness H_{IT}, GPa				
		primary α phase	α phase in eutectic	α phase near SiC_p	α phase near Gr_p	α phase near SiC_p and Gr_p
A356/10SiC	68.8	0.99	1.17	1.01	–	–
A356/10SiC/1Gr	72.6	1.30	1.33	1.21	1.26	1.06
A356/10SiC/3Gr	71.4	1.10	1.18	1.34	1.26	1.11
A356/10SiC/5Gr	55.4	1.03	1.23	1.31	1.00	1.00

Table 1: Macro- and nanohardness values of tested composites

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TRIBOMECHANICAL CHARACTERIZATION OF INDIVIDUAL NANOSTRUCTURES SUPPORTED BY FEM SIMULATIONS

Sergei Vlassov[1,2], Boris Polyakov[1], Leonid Dorogin[2], Mikk Antsov[2], Magnus Mets[2], Mikk Vahtrus[2], Sven Oras[2] and Rünno Lõhmus[2]

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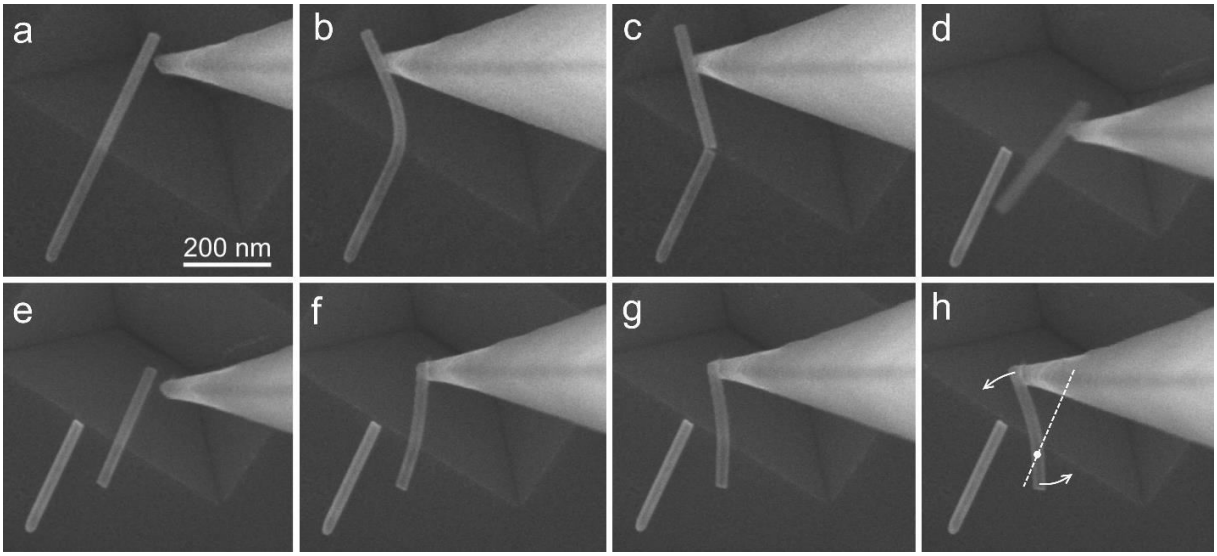
Rapid development of nanotechnology allowed researchers to synthesize a plenty of novel materials and create various nanostructure-based systems with promising applications. However, challenges are related not only to synthesis, but also with subsequent characterization of obtained structures. Due to the small size of the investigated objects, manipulations and measurements are not trivial tasks. If mechanical or tribological characterization of single nanostructures is required, then mainly atomic force microscope (AFM) is used as a manipulation and measurements tool. AFM provides high resolution and accuracy, however it has certain limitations. Main problem is that manipulation and visualization cannot be performed simultaneously. Therefore, there is no real-time visual feedback concerning the behavior of the structure during manipulation, which can lead to partial loss of essential data. In this work, we demonstrate real-time manipulation technique inside a scanning electron microscope (SEM) employed for tribological and mechanical characterization of nanostructures. Strong advantages of the AFM are implemented with visual guidance of the SEM. Different approaches to force measurements are described through the examples on various nanowires and nanoparticles of different geometry. Limitations of the method are discussed. In addition, the use of finite element method (FEM) simulations as support for experimental tribomechanical studies is demonstrated.



Example of mechanical and tribological characterization of ZnO nanowire inside SEM

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ENERGY DISSIPATION MECHANISM ON LAYERED STRUCTURES

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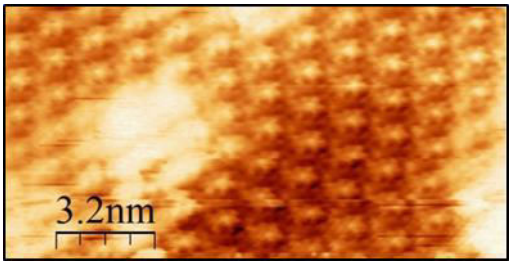
Bodies in relative motion separated by few nanometers gap experiences a tiny friction force [1]. Although nature of non-contact friction is not fully understood yet, it can be measured by highly sensitive cantilever oscillating like a tiny pendulum over the surface [2, 3]. Giant dissipation was reported on $NbSe_2$ surface and associated to nonlinear response of the charge density waves (CDW) [4]. However the problem of friction in similar systems still remains unexplored. Phase transition of TaS_2 between Mott insulating (nearly commensurate CDW) and metallic state (commensurate CDW) depending on the temperature has been reported [5]. It is our interest to observe energy dissipation on TaS_2 and influence of the phase transition on energy dissipation.



CDWs on TaS_2 STM image of CDW on TaS_2 surface. I_t=0.4nA, V_b=10mV

In this study, we observed CDW on TaS_2 by using STM and performed energy dissipation measurement in order to understand the mechanism of energy dissipation on these surfaces due to the tip sample interaction by using pendulum AFM.

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QUANTIFYING MINERAL SURFACE ENERGY BY SCANNING FORCE MICROSCOPY

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Fundamental understanding of the wettability of carbonate formations can potentially be applied to the development of oil recovery strategies in a complex carbonate reservoir. In the present study, surface energies of representative carbonate samples were evaluated by direct quantitative force measurements, using scanning force microscopy (SFM) at submicron scale, to develop a reliable method to predict reservoir wettability. Local adhesion force measurements were conducted on appropriate calcite and dolomite samples and performed in air as well as in the presence of polar and nonpolar fluids. This study demonstrated that, by comparing measurements of adhesion forces between samples of the same mineral in different fluids, it is feasible to determine the surface energy of a given mineral as well as its polar and nonpolar components. The derived values are in agreement with literature. A proof-of-principle protocol has been established to quantify surface energy using SFM-based adhesion measurements. This novel methodology complements the conventional contact angle measurement technique, where surface energy can only be examined at large length scale. The reported methodology has great potential for further optimization into a new standard method for fast and accurate surface energy determination, and hence provides a new tool for reservoir rock wettability characterization [1].

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