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Time	Monday 26	Tuesday 27	Wednesday 28	Thursday 29	Friday 30
8.20 – 9.00	Registration				
9.00 – 9.10	Opening				
9.10 – 9.30	Urbakh	Bechinger	Robbins	Vuletic	Bennewitz
9.30 – 9.50					
9.50 – 10.10	Kuhl	Ma	Riedo	Goldberg	Espinoza-Marzal
10.10 – 10.30					
10.30 – 11.00	*Coffee Break*	*Coffee Break*	*Coffee Break*	*Coffee Break*	*Coffee Break*
11.00 – 11.20	Kisiel	ICTP Lecture by Michael V. Berry	Berkovich	Panizon	Vernes
11.20 – 11.40	Brovko		Schirmeisen	Dietzel	
11.40 – 12.00	Bocquet		Hod	Muser	Meyer
12.00 – 12.20					
12.20 – 14.00	*Lunch*	*Lunch*	*Lunch*	*Lunch*	*Lunch*
14.00 – 14.20	Oğuz	Johannsmann	Franek	Wahl	
14.20 – 14.40	Pawlak	De Wijn		Mandelli	
14.40 – 15.00	Voitchovsky	Poster Session	Zin	Laurson	
15.00 – 15.20			Khomenko		
15.20 – 15.40	Pellegrini		Wiertlewski	Noel	
15.40 – 16.00	Butikova			Yildiz	
16.00 – 16.30	*Coffee Break*	*Coffee Break*	*Coffee Break*	*Coffee Break*	
16.30 – 16.50	Pethica	Guerra	Papastavrou	Perez	
16.50 – 17.10	Sayin	Zheng		Dorogin	
17.10 – 17.30	Sivebæk		COST MC Meeting	Gulseren	
17.30 – 17.50	Spencer	Capozza		Drummond	
17.50 – 18.10		Valtiner			
18.10 – 18.30					
	Welcome Reception (19.00 – 20.30)		Social Dinner (19.30 – 21.30)		

INVITED TALKS

Bechinger C.

Experimental Observation of the Aubry Transition in Colloidal Monolayers

Thorsten Brazda and Clemens Bechinger

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According to the famous prediction of Aubry, static friction of an incommensurate system can completely vanish under certain conditions. For a monolayer of interacting particles, there exists a critical value of the particle-substrate interaction below which the monolayer can set into motion by an infinitesimally small driving force. So far, experimental evidence of this phenomenon has been only obtained for one-dimensional chains of a few atoms exposed to optical potentials [1]. In our experiments we investigate for the first time an extended two-dimensional colloidal crystal containing several thousands of monodisperse particles which are driven across a hexagonal substrate, the latter being created by a laser interference pattern. We observe the disappearance of static friction for non-zero substrate strengths, which is accompanied by marked by the occurrence of finite Novaco-angles. In addition, we find the coexistence of a pinned and a superlubric phase, which suggests the Aubry transition to be of first order in agreement with recent numerical simulations [2].

[1] Bylinskii, A., et al., *Observation of Aubry-type transition in finite atom chains via friction.* Nature Materials, 2016.
[2] Mandelli, D., et al., *Superlubric-pinned transition in sliding incommensurate colloidal monolayers.* Physical Review B, 2015. **92**(13): p. 134306.

Bennewitz R.

Friction and molecular adhesion

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The sliding of a contact requires the breaking of bonds, but also leads to formation of new bonds. Is the energy require to break the bonds all dissipated? Friction force microscopy experiments provide insights into the molecular mechanisms of friction for contacts with a small number of bonds. I will discuss results for friction and adhesion where the tip-sample interaction is controlled by supramolecular guest-host bonds [1]. For low scanning velocities, the bonds are in thermodynamic equilibrium, i.e. the bonds unbind and rebind many times before the contact moves by one molecular distance on the surface. In this situation, one expects zero friction. Zero friction is indeed observed for a stiff attachment of molecules to tip and surface, but finite friction is observed even at low velocities if the molecular attachment is compliant. The results are discussed by comparison with forces measured in pull-off experiments. Molecular simulations clarify the picture of adhesion and friction mechanisms [2]. We show that the force required to break single molecular bonds depends on the cantilever stiffness [3]. Finally, we discuss the role of contact aging in the understanding of molecular friction.

[1] J. Blass, M. Albrecht, B. L. Bozna, G. Wenz, and R. Bennewitz, Nanoscale 7 (2015) 7674.
[2] R. Guerra, A. Benassi, A. Vanossi, M. Ma, and M. Urbakh, Physical Chemistry Chemical Physics 18 (2016) 9248.
[3] J. Blass, M. Albrecht, G. Wenz, Y. N. Zang, and R. Bennewitz, Physical Chemistry Chemical Physics 19 (2017) 5239.

Bocquet L.

Slippery roads

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The question of the hydrodynamic boundary condition of fluids at solid surfaces has entertained the field of fluid transport for most than 20 years. The debate has been quite intense among experimental groups reporting strongly contrasted results. This culminated notably with the measurement of ultra-fast flows in carbon nanotube (CNT) membranes by several groups ten years ago, which pointed to considerable surface slippage and nearly frictionless transport in CNT [1].

In this presentation I will review the main physical mechanisms underlying hydrodynamic slippage, as well as the various experimental results obtained in this domain. This involves in particular slippage on flat surfaces, which highlights the influence of non-wettability. I will also discuss our recent experimental efforts to measure the transport and permeability of individual nanotubes [2,3]. Our experiments reveal diameter-dependent surface slippage in carbon nanotubes, with giant flow enhancements in the smallest tubes [3]. In contrast, their boron-nitride analogues, which have the same crystallinity as CNT, but are electronically different, exhibit no slippage. This points to a hitherto not appreciated link between hydrodynamic flow and the electronic structure of the confining material.

[1] *«Flows in one-dimensional and two-dimensional carbon nanochannels: Fast and curious»*, M. Majumder, A. Siria, L. Bocquet, **MRS Bulletin**, April 2017.

[2] «*Giant osmotic energy conversion measured in a single transmembrane boron-nitride nanotube*», A. Siria, P. Poncharal, A.-L. Biance, R. Fulcrand, X. Blase, S. Purcell, and L. Bocquet, **Nature** 494, 455-458 (2013).

[3] «*Massive radius-dependent flow slippage in singe carbon nanotubes»*, E. Secchi, S. Marbach, A. Niguès, D. Stein, A. Siria and L. Bocquet, **Nature 537** 210 (2016).

Drummond C.

Electro-Responsive Polyelectrolyte-Coated Surfaces

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Most of the studies in friction control have been devoted to improve lubricant design based on novel chemistry or better formulations, combining engineering, know-how and trial-and-error methods. Customarily, walls are considered as confining inert boundaries, with invariable interactions among themselves and with the lubricants. However, considering the surfaces as active components of the system may open avenues for novel functions; appealing applications can be foreseen if the control of the composition and morphology of the surfaces can be tuned in a reasonable time scale. Polyelectrolytes are convenient elementary bricks to build responsive surfaces, given that the polyion chain conformation is very sensitive to different environmental variables. Thus, the state of a typical polyelectrolyte can be controlled by external stimuli or environmental changes, allowing for reversible modifications of the intimate structure of the surface. In this way, active control of the surface properties is possible by adjusting the local molecular conformation of a responsive polyelectrolyte layer. Conformation of polyions can be manipulated by variations in pH or ionic strength. However, chemical variables are in general difficult to control. In addition, the characteristic time of response of molecules to changes of these parameters can be long. In this work we discuss how surface properties can be controlled following a completely different strategy, based on physical methods. We verified that conformation of adsorbed polyelectrolytes can be manipulated using and external electric field, as a consequence of their ionic charge. By dynamically tuning the conformation of the lubricant, fast variation of friction, adhesion and wettability can be achieved. The strong points and limitations of this method of surface properties control will be discussed

Espinosa-Marzal R.M.

Molecular Insight into of Polymer-Ionic Liquid mediated Lubrication

Rosa M. Espinosa-Marzal

University of Illinois at Urbana-Champaign

It is well-known that the fluid-like cushioning layer of solvated polymer brushes effectively reduces friction. The lubrication mechanism relies on the repulsive force of osmotic and steric origin that efficiently separates the two counter-surfaces, thereby hindering polymer chain overlap. As a consequence, a thin film of solvent remains between the two polymer chains providing a plane that is easy to shear, which reduces friction. To fully leverage the lubricating behavior of polymer brushes, a very good solvent is needed to stretch the anchored polymer chains. Ionic liquids (ILs) are considered outstanding solvents, and thus, they could potentially serve as the swelling agent for neutral polymers, and polyelectrolytes. Moreover, they have a low vapor pressure, high viscosity and thermal stability, and higher conductivity and electrochemical stability than other aqueous and non-aqueous solvents, which provides a route to design novel lubricant systems with improved properties for a greater field of applications.

Ionic liquids are known to absorb on many surfaces and to form multi-layer boundary films at the solid-liquid interface. In the absence of tribochemistry, this behavior has been shown to promote low friction compared to lubricant oils under similar conditions. However, thermal fluctuations at soft interfaces, like in case of polymer brushes, are known to disturb the layering of boundary films, and hence, different mechanisms are responsible for the lubrication provided by these films. Based on our studies at the molecular scale, we propose various mechanisms underlying the shear behavior of binary systems composed of polymer films and ionic liquids.

Franek F.

Excellence Center of Tribology: the institution, the highlight topics, and the research roadmap

F. Franek[a,b] and A. Pauschitz[a]

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Almost 15 years ago, the Austrian Centre of Competence for Tribology has been founded in Wiener Neustadt, Austria. The Centre is operated by the privately organised AC2T research GmbH that was built up based on the Austrian Tribology Society (ÖTG, founded 1976). Unique premises enabled the transfer of activities from a working area at the TU Wien and a couple of projects administered by the ÖTG to a dedicated institution for interdisciplinary tribological research. A number of tesserae – determined persons, available engineering expertise, specific knowledge about economic needs and chances of a tribology hot spot in Austria, benevolent officials and, last but not least, public funding contributions – could be completed like a puzzle. Over the years, the Centre could expand to an internationally visible institution with more than 100 scientists, technical and administrative staff members and an extensive infrastructure mainly focused on materials, surface and lubricant analyses, tribometrology and computer-aided engineering tribology.

The mission of ACÇT is implemented in several research activities, to a certain extent embedded into the Austrian COMET program, a national funding initiative for basic-oriented applied research and open for international participation. The research projects put into practice the holistic approach and are executed by teams from eight “research pools” and managed by one of four “research areas”, viz. Lubricants and Interface Mechanisms, Wear Processes and Wear Protection, Friction Surface Phenomena and Tribodiagnostics and, Computation and Experimental Simulation. The “window for observation” is particularly important and mostly pertains to significant, relevant phenomena on micro or nano level and, e.g. status and changes of (micro)structures of surfaces and of near-surface zones, adsorption and chemical reactions of and caused by lubricating matter, generation and transport of wear particles and contaminations, considering (nano)rheological effects of lubricant flow.

In the present talk, an overview will be given of the orientation and the scope of the Centre as well of some selected research topics of ACÇT projects of scientific and strategic interest to understand, quantify and influence wear mechanisms and to improve friction behaviour of systems.

A focus is laid on the high resolution quantification of wear by radioisotope concentration (RIC) method under several lubrication conditions. Complementary methods like ellipsometry enable the study of formation and duration of tribofilms. Additional information on the wear process, like early detection of incipient material damage in tribological contacts, can be derived from determining the size distribution of sub-µm metallic wear particles in the lubricating oil.

Subsurface modification/damage of lab-scale modelled rolling contact on rails were studied by a tribological wheel-rail model test set-up combined with early-damage analysis which were done for pure pearlitic and ferritic/pearlitic rails mainly by electron backscatter diffraction (EBSD).

Self-tuning properties of multifunctional surfaces are addressed by in-situ generation of W-S tribofilms using functionalized surfaces and green additives, the synergy of both creates an in-situ TMD (Transition Metal Dichalcogenides) tribofilm triggering a considerable drop of CoF.

An example is also given for a Molecular Dynamics (MD) simulation approach to study grinding and polishing processes which enables a quantitative evaluation of wear volume and real contact zone by using multiple abrasives. The formation of a tribo-layer can be explored for an ultra-fine pearlite component (combining ferrite matrix with cementite lamellae).

Goldberg R.

Liposomes as a platform for lubrication and for drug delivery: utilizing the hydration lubrication paradigm in vitro and in-vivo

Ronit Goldberg, Weifeng Lin and Jacob Klein

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Liposomes are vesicles whose walls are composed of a closed phospholipid membrane whose size ranges from tens of nanometers to several microns and more. Previous studies indicated that phosphatidylcholine (PC) liposomes may act as extremely efficient lubricants at physiologically high pressures in aqueous media. Small unilamellar vesicles (SUVs) of hydrogenated soy phosphatidylcholine (HSPC) lipids self-assemble in close-packed layers on solid surfaces, and reduce the coefficient μ of sliding friction between them down to values μ of $O(10^{-4} - 10^{-5})$, at pressures up to ca. 12 MPa (ca. 120 atmospheres). Such low values of sliding friction at these physiologically-high pressures have not been attained with any boundary lubricants. We attribute this low friction to hydration lubrication by the highly-hydrated phosphocholine head-groups exposed at the vesicle walls, further stabilized against high pressures by the close-packing and by the rigidity of the liposomes (which are in their gel phase). Further experiments measuring friction between synthetic surfaces (plastic and hydrogels) and natural surfaces (cartilage and tendons) demonstrate that PC liposomes can reduce dramatically the friction in different systems. This suggests that intra-articular administration of PC liposomes as lubricants may alleviate osteoarthritis; interestingly, this may be combined with the fact that liposomes are also widely-used drug delivery vehicles, as they can encapsulate a wide range of drug molecules. However, a big disadvantage common to all particulate carriers is that following administration, they are rapidly removed from the body, mainly by the cells of the mononuclear phagocyte system. It is known that the use of phosphatidylethanolamine with a covalently attached polyethylene glycol (PE-PEG) incorporated in liposomes results in a long circulation time and high retention of the PEGylated liposomes compared with the pure (non-PEGylated) liposomes. We use a novel polymer, synthesized to incorporate the hydration lubrication concept, in order to replace and improve PEG both for lubrication and retention, and tested this approach *in vivo*. The rational was that the hydrated molecules may deceive the immune system that will first recognize water of hydration rather than the liposome membrane, resulting in an increased retention time. When our new liposomic-vehicles were intra-articularly injected into mice knee joints we found an increase of the vesicles' retention half-life of about 7-fold (ca. 600% increase in retention time) compared with the state-of-the-art PEGylated liposomes. This holds promise for long-lived intra-articular lubricants as well as drug-delivery vehicles with exceptionally-long *in vivo* retention times.

Hod O.

Modeling Interlayer Interactions in Layered Materials

Oded Hod

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Sackler Faculty of Exact Sciences
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In the past two decades low dimensional layered nano-materials have been at the forefront of scientific research. Owing to a variety of novel outstanding physical properties graphene, hexagonal boron nitride (*h*-BN), and transition metal dichalcogenides (TMDC) hold great promise for becoming key components in the next generation of advanced electronics, strong lightweight materials, and friction reducing technologies. The interlayer interactions in these materials play a central role in shaping their mechanical and electronic properties. In my lecture, I will present a new methodology for modeling these interactions using specially tailored classical force-fields. The computational capabilities of the developed methodology will be demonstrated via several applications addressing the structural, mechanical, and tribological properties of layered materials including the super-structure of graphene/*h*-BN heterojunction, which has been shown to alter graphene electronic properties, and the occurrence of circumferential faceting in double-walled nanotubes. Then I will turn to describe interlayer electrical conductance across a twisted graphene interface, where I will show the strong correlation between interlayer structural commensurability and cross-layer electrical transport.

Polymer Brushes in Restricted Geometries

Tonya Kuhl

University of California at Davis

Polymer molecules at solid or fluid interfaces have an enormous spectrum of applications in a wide variety of technologies from lubrication of mechanical surfaces to the synthesis of biocompatible interfaces. Over the past two decades, neutron reflectivity measurements have become a powerful tool for measuring the conformations of ultra-thin polymer layers at interfaces, however the structure of solvated polymer brushes under confinement and/or shear has remained elusive due to the inherent difficulties in measuring thin-film properties. In this talk, I will present novel neutron reflectivity measurements of the structure of opposing polymer brushes as a function of confinement. I will compare these results to the structure of polymer brushes at a single interface as well as to high precision surface force apparatus measurements of the force required to compress and shear polymer brushes. Although good agreement can be obtained between physical experiments, simulations and theory under low to moderate grafting densities, ultra-high density brushes offer new challenges and behavior that has not yet been fully addressed. Significantly, the experimental relaxation time of ultra-high density brushes formed by grafting from methods (ATRP) was found to be at least four orders of magnitude longer than that predicted by the Rouse model resulting in enormous hysteresis during compression. Yet, the shear performance of such brushes demonstrated excellent lubricity under compressions down to 35% solvent content. The findings are consistent with a reduction in solvent quality with compression leading to shrinkage or collapse of the brush under high compression (increasing polymer concentration), while still maintaining a region of well solvated chains in the overlap region between opposing brushes. Together, the results suggest that compression hysteresis is primarily due to intra-brush entanglements and collapse of the brush layer rather than inter-brush entanglements and brush–brush interpenetration. The importance of the ultra-high density, ultra-polydisperse brushes yielding favorable lubrication properties is that a highly durable lubricating layer can be formed from a “realistic” system versus the more ideal, monodisperse systems that have been primarily studied in the past.

Lubricated friction at the nanoscale: insights from molecular dynamics simulations and machine learning

Lasse Laurson

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Lubricated friction is an inherently multi-scale problem where details of the atomic scale interactions together with larger-scale effects such as surface morphology determine the macroscopic frictional response of the system. Here, I will give an overview of our recent efforts to understand some of the properties of nanoscale systems where thin lubrication layers are confined by parallel surfaces in relative sliding motion, using classical molecular dynamics (MD) simulations.

First, I discuss the effect of different types of surfaces confining thin layers of water, considering as example surfaces hydrophilic mica and hydrophobic graphene [1]. We observe stick-slip dynamics for thin water films confined by mica sheets, involving periodic breaking-reforming transitions of atomic-scale capillary water bridges formed around the potassium ions of mica. However, only smooth sliding without stick-slip events is observed for water confined by graphene, as well as for thicker water layers confined by mica, illustrating how atomic-scale details affect the wettability of the confining surfaces and consequently control the presence or absence of stick-slip dynamics in nanoscale friction.

Second, I focus on lubricants consisting of liquid crystal molecules (6CB), which have recently emerged as potential candidates for next generation lubricants, considering also various mixtures of 6CB and hexane [2]. Our results demonstrate the key role of the structure of the mica surfaces in determining the nature of sliding friction with monolayer lubricants, including the presence or absence of stick-slip dynamics. For thicker lubrication layers the surface structure becomes irrelevant, but friction may still be controlled by tuning the relative concentrations of 6CB and hexane in the mixture. Lubrication properties of 6CB monolayers are insensitive to applied fields due to strong confinement effects, but significant friction reduction by external electric fields is demonstrated to be feasible for thicker 6CB layers.

Finally, I describe our recent attempt of applying machine learning (ML) to infer the relation between the composition of lubricants and their performance [3]. To this end, we first use MD simulations to generate a database containing the frictional response of a large set of toy polymer-like fluids characterised by different random chain length distributions of the molecules. We then model the fluid-friction relation by a Bayesian neural network, trained to reproduce the results for a training set of fluids. We discuss the challenges arising due to the inhomogeneous distribution of data, as well as the prospects of applying ML methods to develop lubricants with optimal properties.

[1] W. Chen, A. S. Foster, M. J. Alava, and L. Laurson, Stick-slip control in nanoscale boundary lubrication by surface wettability, Phys. Rev. Lett. 114, 095502 (2015).

[2] P. Kumar Jana, W. Chen, M. J. Alava, and L. Laurson, submitted

[3] M. A. Zaidan, F. F. Canova, L. Laurson, and A. S. Foster, Mixture of Clustered Bayesian Neural Networks for Modeling Friction Processes at the Nanoscale, J. Chem. Theory Comput. 13, 3–8 (2017).

Ma M.

Controllable robust superlubricity on microscale

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Superlubricity is a state where the friction between two mono-crystalline surfaces in contact is vanishing. Achieving controllable robust superlubricity on large scale is crucial for its practical application. Here we report such states observed experimentally in microscale graphite flake homojunction and graphite–hexagonal boron nitride heterojunction. For graphite flake homojunction, we find different friction-velocity dependence at different temperature, and an interesting wear phenomenon at ambient condition. For graphite-hexagonal boron nitride heterojunction, we find a superlubric state which is robust against rotation, normal pressure, atmosphere and wear. Our results provide experimental basis for the application of superlubricity on microscale, and shed insight on the way towards macroscale superlubricity.

Meyer E.

Graphene Nanoribbons and Polymeric Chains Sliding on Au(111)

E. Meyer[1], R. Pawlak[1], S. Freund[1], T. Meier[1], U. Gysin[1], T. Glatzel[1], R. Joer[1]
and S. Kawai[1,2]

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2 MANA, National Institute for Materials Science 1-1 Namiki, Tsukuba, Ibaraki, 305-0044, Japan.

Manipulative force microscopy uses the probing tip to pick up a single molecule or nanoribbons and to perform a number of experiments with the attached molecule. Either lateral or vertical manipulations can be performed, where a number of parameters, such as velocity, temperature or orientation angle, are available. An example is given by the pulling of polymeric chains on Au(111) [1], where the detachment of the chain leads to oscillations of the normal and lateral forces. The comparison with the model yields the adhesive energy per subunit of the molecular chain. Lateral manipulation gives insight into the movement of one dimensional chains on surfaces. An example with potential for application is the pulling of graphene nanoribbons across an Au surface [2]. In this case, superlubricity conditions were found. The movement in the [-101] direction shows a rather high degree of incommensurability. The graphene ribbon shows quite high stiffness, which even allows us to reverse the sliding direction with small hysteresis. A second class of experiments is to pick up a single molecule and to investigate the influence of internal degrees of freedom during lateral and vertical manipulations [3]. In the case of a porphyrin derivative it is the motion of a di-cyanophenyl side group, which determines the mechanical response. This method is also useful to observe inhomogeneities on the surface, e.g. the elbow sites of the herringbone reconstruction.

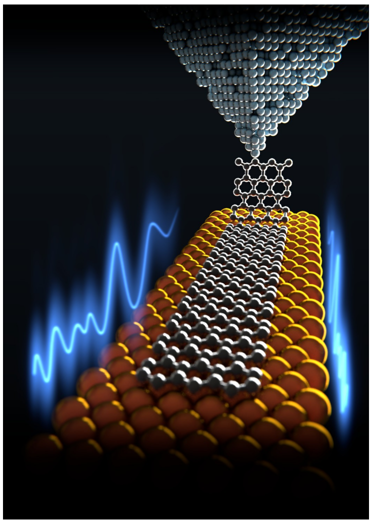

Fig: Graphene nanoribbon is pulled across an Au(111) surface by force microscopy.

[1] S. Kawai, M. Koch, E. Gnecco, A. Sadeghi, R. Pawlak, Th. Glatzel, J. Schwarz, S. Goedecker, S. Hecht, A. Baratoff, L. Grill, and E. Meyer, Proc. Natl. Acad. Sci. USA, 111, (11), 3968–3972 (2014).
[2] S. Kawai, A. Benassi, E. Gnecco, H. Söde, R. Pawlak, X. Feng, K. Müllen, D. Passerone, C. A. Pignedoli, P. Ruffieux, R. Fasel, E. Meyer
Science, 351, (6276), 957 (2016).
[3] R. Pawlak, W. Ouyang, A. E. Filippov, L. Kalikhman-Razvozov, S. Kawai, T. Glatzel, E. Gnecco, A. Baratoff , Q.-S. Zheng, O. Hod, M. Urbakh, E. Meyer, ACS Nano, 10, 713-722 (2016).

Meeting the (Tribology Letters) Contact-Mechanics Challenge

Martin H. Müser

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Contact-mechanics is a thriving field with various schools each claiming to be valid. To ascertain the relative merit of different methods, a mathematically well-defined contact-mechanics problem was posted. Its accurate solution necessitated either access to efficient codes and large computers, or a valid theory simplifying the problem, or some other out-of-the-box idea. Thirteen different groups participated in the challenge [1]. Quite complementary approaches were pursued. They ranged from brute-force computing, Persson theory, and Greenwood-Williamson inspired models. Even real-laboratory experiments and all-atom simulations of a scaled-down problem were conducted. In this talk, some highlights of the results will be presented.

[1] Martin H. Müser, Wolf B. Dapp, Romain Bugnicourt, Philippe Sainsot, Nicolas Lesaffre, Ton A. Lubrecht, Bo N. J. Persson, Kathryn Harris, Alexander Bennett, Kyle Schulze, Sean Rohde, Peter Ifju, W. Gregory Sawyer, Thomas Angelini, Hossein Ashtari Esfahani, Mahmoud Kadkhodaei, Saleh Akbarzadeh, Jiunn-Jong Wu, Georg Vorlaufer, András Vernes, Soheil Solhjoo, Antonis I. Vakis, Robert L. Jackson, Yang Xu, Jeffrey Streator, Amir Rostami, Daniele Dini, Simon Medina, Giuseppe Carbone, Francesco Bottiglione, Luciano Afferrante, Joseph Monti, Lars Pastewka, Mark O. Robbins, and James A. Greenwood, *Meeting the Contact Mechanics Challenge*, Tribol. Lett. (submitted).

Papastavrou G.

Controlling and Manipulation Surface Forces by Electrochemistry

Georg Papastavrou

Physical Chemistry II, University of Bayreuth, Germany

Electrochemistry does not only allow to follow charge transfer process at electrodes but also to tune the surface and in particular the diffuse layer properties of an electrode. By modifying the surface of gold electrodes by an additional self-assembled monolayer of thiols it is possible to tune the surface chemistry of a modified electrode in a defined manner. Thereby, not only the electrochemical potential at the electrode surface can be varied but also surface properties such hydrophobicity or presence of ionisable groups. These independent variation is not only interesting to study effects like charge regulation but also a novel approach to study adsorption processes.

The diffuse layer properties and adhesive properties of the modified electrodes can be determined by direct force measurements with the atomic force microscope. In order to provide a defined interaction geometry, we primarily use the colloidal probe technique, which is based on attaching a colloidal particle to the end of an AFM-cantilever. The diffuse layer properties of this colloidal probe can be determined unambiguously from symmetric sphere/sphere measurements. Hence, it is possible to extract the diffuse layer properties of the electrode in function of the applied potential by fits to the full Poisson-Boltzmann equation, where we take also charge regulation effects into account.

The adhesion of colloidal objects can be tuned by means of an external potential. A detailed analysis shows that primarily long-ranged electrostatic interactions are responsible for the observed changes of adhesion in function of the applied potential. By contrast, changes in the interfacial wetting properties with potential (Lippmann equation) can be safely neglected. Based on these studies we present a first proof-of-concept for micromanipulation based on potentiostatic control of the adhesive properties. Additional examples that will presented include the effect of ion adsorption on interaction forces, the control of adsorption phenomena by external potentials and scanning electrochemical force microscopy.

[1] Papastavrou, G. Combining Electrochemistry and Direct Force Measurements: From the Control of Surface Properties Towards Applications. *Colloid Polym Sci* **2010**, *288*, 1201.
[2] Rentsch, S.; Siegenthaler, H.; Papastavrou, G. Diffuse Layer Properties of Thiol-Modified Gold Electrodes Probed by Direct Force Measurements. *Langmuir* **2007**, *23*, 9083.
[3] Kuznetsov, V.; Papastavrou, G. Adhesion of Colloidal Particles on Modified Electrodes. *Langmuir* **2012**, *28*, 16567.
[4] Kuznetsov, V.; Papastavrou, G. Ion Adsorption on Modified Electrodes as Determined by Direct Force Measurements Under Potentiostatic Control. *J Phys Chem C* **2014**, *118*, 2673.

Riedo E.

Sub-Å-resolution elasticity and friction in 2D Van der Waals materials

Yang Gao[1,2], Si Zhou[1], Daniel Nélias [3], Claire Berger[1], Walt de Heer[1],
Angelo Bongiorno[1,4] and Elisa Riedo[1,2]

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Two-dimensional (2D) materials, such as graphene and MoS_2, are a few-atomic-layer thick films with strong in-plane bonds and weak interactions between the layers. The in-plane elasticity has been widely studied in bending experiments where a suspended film is deformed substantially; however, little is known about the films' elastic modulus perpendicular to the planes, as the measurement of the out-of-plane elasticity of supported 2D films requires indentation depths smaller than the films' interlayer distance.

Here, we present a new method to perform sub-Å-resolution indentations to measure the perpendicular-to-the-plane elasticity in 2D materials and nanotubes [1], and its implications for graphene and graphene oxide films. This method, called Å-indentation goes beyond the standard nanoindentation approach and allows for high resolution elasticity measurements of films that are atomically thin and extremely stiff. Our indentation data, combined with semi-analytical models and density functional theory are then used to study the perpendicular elasticity of a few-layers thick graphene and graphene oxide films. We find that the perpendicular Young's modulus of graphene oxide films reaches a maximum when one complete water layer is intercalated between the graphitic planes. This non-destructive methodology can map interlayer coupling and intercalation in 2D films.

Furthermore, we will discuss our recent work on the interplay between number of layers, structure, defects and friction in MoS_2 films.

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Robbins M.O.

Scale Dependence of Contact and Friction from Atomic to Macroscopic Scales

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Friction and adhesion are inherently complex multiscale problems. The forces between surfaces come from opposing atoms that are separated by less than a nanometer, but the number and location of these atoms is determined by surface topography and subsurface elastoplastic deformation on nanometer to millimeter scales. This talk will explore the interplay of surface structure and substrate elasticity in determining contact area A and friction F as dimensions increase from atomic to macroscopic scales. Combining molecular dynamics with a Greens function technique allows study of contacts with dimensions of micrometers while resolving atomistic interactions at the surface.

First contact of rough spherical tips is described. For small tips and high loads the contact area follows predictions for contact of smooth spheres. For large tips and low loads, contact area is proportional to load. Simple analytic formulae capture the crossover between these regimes for nonadhesive and adhesive contacts. Next the friction in single-asperity contacts is studied. When elasticity is neglected, most bare contacts exhibit superlubricity: $F \propto A^x$ with $x \leq 0.5$. Friction and area are only proportional ($x=1$) in the rare case of commensurate surfaces with the same period and orientation. For crystalline surfaces we find that interfacial dislocations lead to quantitative deviations from rigid substrate scaling when the contact radius a is greater than the interfacial dislocation core width b, which scales inversely with the shear modulus. For $a>b$, the ratio F/A for commensurate surfaces drops, while F/A rises for incommensurate surfaces. In the limit of large a, all crystalline surfaces have F/A near the Peierls stress for dislocation motion. Dislocations do not form for amorphous tips but there is still a crossover to linear scaling of F with A for compliant surfaces. Moreover the limiting shear stress is similar in magnitude to the Peierls stress. For all tip geometries the limiting shear stress decreases exponentially with the ratio of stiffness to local interfacial shear strength.

Imitating Cartilage with Polymers

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Structures involving brushes on soft surfaces [1, 2] are typical for natural lubricated systems, such as the cornea, and the lining of the gut. Cartilage has a layered, gradient structure, right up to the articular surface, where it is widely believed to terminate in a low-modulus, gel-like layer surmounted by loose chains.

The structure of cartilage is the inspiration for our current project, in which we are growing polymer gels and brushes by means of radical polymerization, and incorporating polyelectrolytes into the gels to mimic the charged proteoglycan aggregates that are trapped within the collagen matrix of the cartilage (Figure 1).

In addition to the many synthetic challenges of this project, an analytical challenge is the measurement of the mechanical properties of brush-covered soft systems. A novel, 2-step nano-indentation approach has been devised that unambiguously allows the detection of the outer surface, as well as independent dynamic measurements of the moduli of both brush and gel layers.

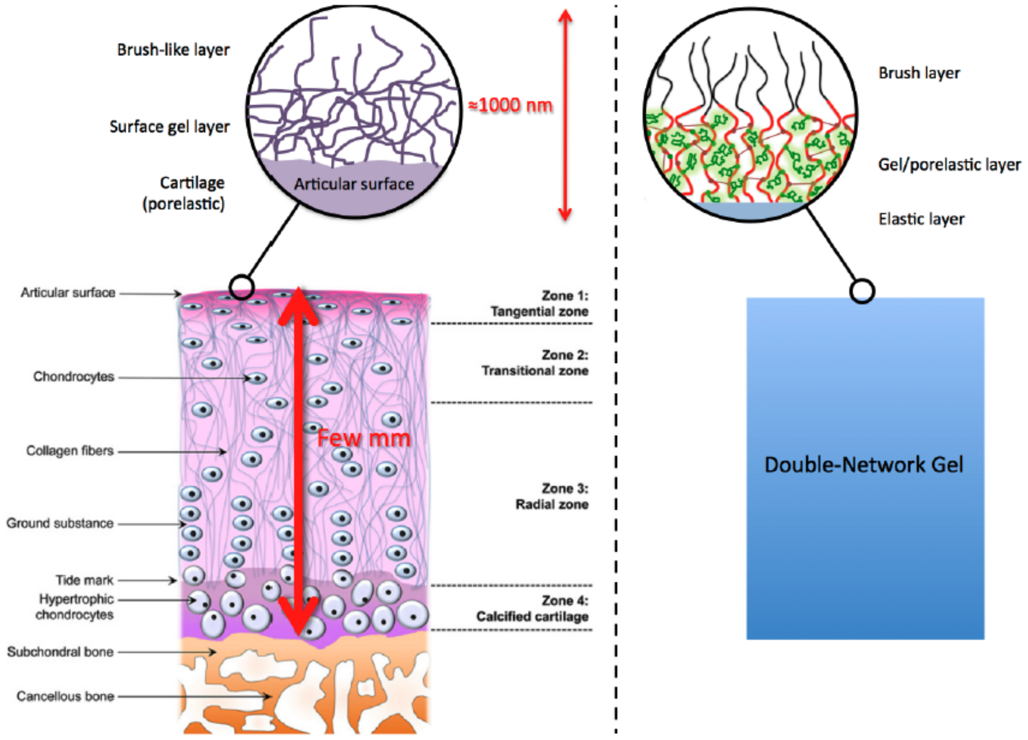

Figure 1: Left: Structure of cartilage, Right: Polymer imitation of cartilage

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Urbakh M.

Electrotunable Friction with Ionic Liquid Nanoscale Films

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Room temperature ionic liquids recently attracted a lot of scientific attention as the flexibility in the choice of the cation/anion molecules allows the properties of the liquid to be fine-tuned. The behavior of ionic liquids in confined geometries is of great interest for different fields, ranging from biological systems to super-capacitors, micro/nano-fluidic, and lubrication. Ionic liquids form layered structures at surfaces, yet it is not clear how this nano-structure relates to their lubrication properties.

Using nonequilibrium molecular dynamics simulations and coarse-grained models of ionic liquids, we have investigated a relation between measured friction forces and structure of confined ionic liquids under shear. We show that the electric field induces significant structural changes in the film, leading to dramatic modifications of the friction force. The impact that the shape and the intramolecular charge distribution of the ions have on the electrotunable friction with ionic liquid nanoscale films is discussed. Comparison of the present work with previous studies using different models of ionic liquids indicate that the phenomenology presented here applies to a wide range of ionic liquids. In particular, the electric-field-induced shift of the slippage plane from the solid−liquid interface to the interior of the film and the nonmonotonic variation of the friction forcé are common features of ionic lubricants under strong confinement. We demonstrate that the molecular structure of the ions plays an important role in determining the electrostriction and electroswelling of the confined film, hence showing the importance of ion-specific effects in electrotunable friction. The effect of water on friction in ionic liquids is also discussed. These findings open new pathways for lubricant design.

Valtiner M.

In-situ tracking of the dynamic structure evolution in nanometer confined liquids by combining X-Ray Reflectivity and white light interferometry in a surface forces apparatus

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Liquids that are confined between solid down to the nm range exhibit molecular ordering that finds great importance in the field of friction, lubrication or energy conversion. Thus, a detailed knowledge of the structure on the molecular scale of a confined liquid is of great interest for fundamental and applied sciences. How this structuring of a confined fluid reacts on external triggers such as sliding of surfaces against each other, humidity, or change of applied confining stresses is notoriously hard to measure in experiment. Here, we will discuss how we experimentally provide both structural information as well as a precisely controlled liquid confinement down to the nm level, and that under dynamically changing conditions. For this, we combined the Surface Force Apparatus (SFA) which allows both quantification of applied forces and generation of nano confined well-controlled gaps between two opposing surfaces based on optical interference, and X-Ray Reflectivity that can determine the crystallographic structure of confined fluids on a molecular scale.

A pore with a mm2 area and a precisely controlled heights ranging from10 to 100s of nm of a confined model liquids could be realized. We then also applied dynamic forces through compression and decompression, as well as lateral sliding cycles of the confined liquid between two opposing surfaces. So far, we were able to demonstrate the feasibility of this X-SFA, making this a novel and interesting setup for studying confined fluids under dynamic compression and also during dynamic sliding.

Vernes A.

Multiscale computational tribology

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Tribological processes, e.g. friction and wear, are multiscale phenomena in their nature, i.e. hierarchical in length and time. Therefore tribological systems can be realistically modelled/simulated only in a multiscale fashion, namely by coupling various computational methods, which are highly accurate on their typical length/time scales. Main computational parts of such a multiscale tribological calculation are based on quantum mechanics (QM), molecular dynamics (MD), continuum mechanics (CM) and multibody system dynamics (MBSD), respectively. Although length and time scales overlap to some extent when passing from a computational part to the immediately next one, the main challenge of the multiscale computational tribology still remains the coupling between different levels of modelling.

In the present talk, an overview will be given on serial coupling schemes developed at AC²T over the years together with their manifold tribological applications. Namely, it will be shown that some of well-established approaches and known numerical methods can be not only extended and used to understand important tribological mechanisms on their relevant time/length scales, but they can be also combined into new schemes to cover hierarchical aspects of various tribological processes.

Voitchovsky K.

Lubrication and viscoelastic properties of liquids confined between nano-asperities

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The dynamical properties of nano-confined liquids play an important role in countless systems, ranging from transport in protein channels and pores to nanofluidics-based technologies such as 3D printing, water purification, single molecule detectors, lab-on-chip technology and controlled lubrication. In most real life systems, the confined liquid is not pure, but composed of a mixture of molecules and ions, typically sheared by force flow in nano-channels or by confinement between moving solids. Due to the small size of width of the confining region, the behavior of a given system can be considerably influenced by its molecular-level details, from the exact confining geometry, to the chemical composition of the surfaces, the presence of impurities as well as the measurement itself.

Here atomic force microscopy (AFM) is used with ~1 nm vertical or lateral oscillations amplitudes to probe both the molecular organisation [1] and the viscoelastic properties of liquids sheared between a nanometre size tip and various surfaces [2, 3]. The measurements locally probe a small number of molecules, allowing work on non-ideal interfaces. We explore the influence of parameters such as temperature, pH, liquid composition, solid chemistry and shearing parameters on the viscoelastic properties of aqueous solutions involving different types of ions. The results show a non-Newtonian response of the liquid, with the behaviour (shear-thinning or -thickening) depending on the chemistry of the confining surfaces. Ions act as lubricants, reducing the friction force and the elastic response of the water according to their specific hydration properties. The spatial and temporal scales of the measurements also play an important role, with different regimes suggesting mesoscale effects that involve multiple ions [4] and group dynamics [5]. Group effects and molecular clustering also appear to play a dominant role for the viscoelastic and lubrication properties of organic mixtures of model lubricants [3].

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Vuletic V.

Stick-slip friction studied with trapped ions

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Stick-slip friction occurs on many different length scales down to the nanoscale. To test long-standing atomistic models of friction processes, we have implemented a synthetic nano-friction interface using laser cooled ions subject to the periodic potential of an optical standing wave [1]. We show that stick-slip friction can be tuned from maximal to nearly frictionless via arrangement of the ions relative to the periodic potential, and that friction at the nanoscale can substantially differ from the simple phenomenological laws observed at the macroscale [1,2]. We also establish a direct link [3] between Aubry's structural transition [4] for an infinite chain in an incommensurate periodic potential, and the vanishing of friction in nanocontacts (superlubricity) [5]. I will also present results on stick-slip friction in a multistable potential, and discuss the relation between kinks and superlubricity.

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Wiertlewski M.

Manipulating fingertip friction via partial ultrasonic levitation

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When touched, a glass plate excited with ultrasonic transverse waves feels notably more slippery than it does at rest. To study this phenomenon, we use frustrated total internal reflection to image the asperities of the skin that are in intimate contact with a glass plate. We observed that the load at the interface is shared between the elastic compression of the asperities of the skin and a squeeze film of air. Stroboscopic investigation reveals that the time evolution of the interfacial gap is partially out of phase with the plate vibration. Taken together, these results suggest that the skin bounces against the vibrating plate but that the bounces are cushioned by a squeeze film of air that does not have time to escape the interfacial separation. This behavior results in dynamic levitation, in which the average number of asperities in intimate contact is re- duced, thereby reducing friction. This improved understanding of the physics of friction reduction provides key guidelines for designing interfaces that can dynamically modulate friction with soft materials and biological tissues, such as human fingertips.

Robust Wearless and High Speed Sliding

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Zero wear is one of the most crucial features of superlubricity. It brings a fantastic character to the moving parts which may improves the motion precision greatly and prolong the parts lifetime substantially. Here we report the elimination of wear between microscale highly-oriented pyrolytic graphite and diamond like carbon over a distance of 1,000,000m and a speed of 1.5m/s under ambient condition. Thermal monitoring, Raman spectroscopy analysis and AFM were used, and wear were not detected under these characterization. We find that this wear-free phenomenon is attributed to the weak van der Waals interaction between the two surfaces which are atomic scale flat. These findings promise many applications of superlubricity where ultra-long wearless and high speed sliding are required, including hard disks, electric brushes, and high speed railway pantograph.

CONTRIBUTED TALKS

Estimation of surface corrugation energy amplitude from friction force microscopy measurements of NaCl in ethanol using the Prandtl-Tomlinson model

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Friction force microscopy (FFM), usually performed under ultra-high-vacuum (UHV) conditions, met another operative methodology in recent years, where the measurements were performed in ambient surroundings. In such experiments, the interaction between a sharp nanotip scanning a solid surface under normal loads is recorded by measuring the resulting lateral forces. Here we use the Prandtl-Tomlinson framework to estimate the amplitude of the corrugation potential from FFM measurements of NaCl submerged in ethanol. Ethanol was selected for the liquid media due to the neglible solubility of NaCl in it. The surface potential amplitude scales with the applied normal loads. Furthermore, we show that this scaling is in good agreement with data obtained for NaCl measured under UHV conditions.

External tuning of the spin state of oxygen vacancies at strontium titanate surfaces

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Among the wealth of optical, electronic and magnetic phenomena induced in strontium titanate ($SrTiO_3$) bulk or at its surface by vacancies or dopants, oxygen-vacancy-induced magnetism remains one of the most studied yet still one of the least understood ones. Here we use density functional theory to explore the possibility of dynamically switching the multiplet state of an oxygen vacancy or a vacancy cluster at ideal and reconstructed $SrTiO_3$ surfaces by external stimuli such as charge injection, electric bias or tip-induced force fields. We relate the mechanism responsible for the change in the spin state to charge redistribution at the vacancy site. Since each state change should imply, as for a quantum dot, a dissipation channel for the external agent, these ideas can be tested experimentally, e.g. within the scope of atomic force microscopy at low temperatures.

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Synthesis and Characterisation of ZnO-WS_2 Nanowires, a Model Material for Nanotribology and Manipulation

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Core-shell nanowires (NWs) are modern type of axially heterostructured nanomaterials intensively explored during last decades. Finding an adequate combination of core and shell materials allows a significant improvement of electrical, mechanical and optical properties of NWs.

Zinc oxide (ZnO) is among the most thoroughly explored NW material due to simplicity of it synthesis and a number of beneficial properties [1]. WS_2 is widely used as a lubricant additive [2].

ZnO/WS_2 core-shell nanowires were produced in three steps:

1) ZnO NWs were grown on a SiO_2/Si(100) wafer by a vapour transport method;

2) ZnO NWs were coated by a layer of a-WO_3 using reactive DC magnetron sputtering of metallic tungsten target in mixed Ar/O_2 atmosphere;

3) ZnO/WO_3 NWs were annealed in sulphur atmosphere to convert a-WO_3 into WS_2, followed by heating in inert atmosphere to sublimate the remaining WO_3.

The morphology and phase composition of synthesized ZnO/WS_2 core-shell nanowires were confirmed by scanning and transmission electron microscopy (SEM and TEM), micro-Raman and photoluminescence spectroscopy. The thickness of WS_2 shell varies in the range of 2 to 5 monolayers. Measured interlayer distance is about 6.0 to 6.7 Å. Interplanar distance measured in ZnO/WS_2 nanowires equals to 2.8 Å.

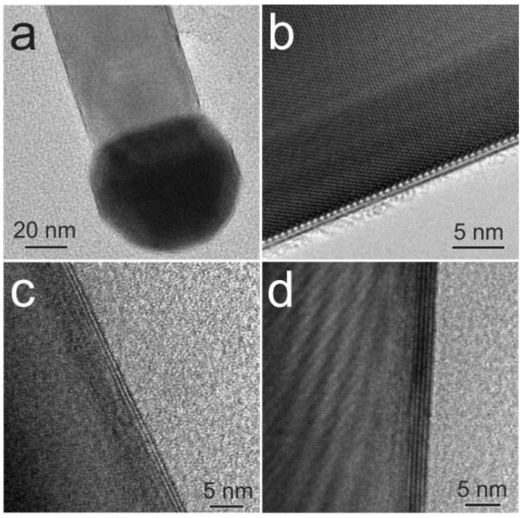

Fig. 1. TEM images of ZnO/WS2 core-shell nanowires at low (a) and high magnifications (b-d). Gold nanoparticle can be observed at the end of the nanowire (a). WS_2 layers are represented as black lines in the surface of ZnO NW [3]

Qualitative agreement in estimate of inter-planar interface distance has been found while comparing experimental and theoretical results that could explain strong adhesion of WS_2 nanolayer to ZnO substrate.

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Layering, glass formation and entropy evolution during squeezout of a model confined ionic liquid (*)

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A potential interest of ionic liquids acting as boundary lubricants is the possibility to tune their squeezout and friction properties through charging of the confining plates. We recently introduced a "tailed model" ionic liquid, rich enough to include some molecular rotation and directionality, but simple enough to enable a dynamical study of friction at variable charging [1], and also study of thermodynamic variables during adiabatic squeezout [2]. The latter includes the calculation, by direct integration of the solvation force, of the solvation enthalpy [2], as well as, at leat in in principle, of the solvation entropy [3] as a function of the confined liquid film thickness. We are conducting fresh simulations which yield the entropy and the internal energy of solvation, and their layering oscillations during squeezout. The behavior of these two quantities may vary from conspiring to complementary in connection with structuring and with changes of molecular tail direction associated with thickness, and with the magnitude and sign of charging. In some cases an entropy drop takes place during squeezout in connection with glass formation, giving rise to a smooth repulsive part of the total interplate enthalpy.

(*) Work sponsored by ERC MODPHYSFRICT, Contract N. 320796

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How square ice helps lubrication

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The combination of water with graphite or graphene is under active investigation in several fields for a number of reasons. In the field of tribology, it is of interest due to the action of graphite powder as a solid lubricant, which is far more effective under humid conditions than in vacuum or dry air. This is opposite to the case for other solid lubricants, such as WS_2 and MoS_2 [1]. Moreover, water alone is a poor lubricant, due to its low viscosity-pressure coefficient. While suggestions have been made as to the reason behind water's beneficial effects on graphite as a lubricant [2], this effect is not yet understood.

We use atomistic molecular-dynamics simulations to investigate equilibration of water confined between graphene sheets over a wide range of pressures. We demonstrate that, under the right sliding conditions, square ice can form in an asperity, and that it is similar to cubic ice VII and ice X. We find that thermal equilibration of the confined water is hindered at high pressures. We simulate sliding of the square ice on atomically flat graphite and find extremely low friction due to structural superlubricity. The conditions needed for this equilibration correspond to low sliding speeds, and we suggest that the ice observed in experiments of friction on wet graphite [3, 4] is of this type.

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Universal Contact Ageing Mechanism revealed by Stick Slip Measurements of Sliding Nanoparticles

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On the macroscale, static and sliding friction are typically experienced as two very distinct phenomena. However, they can be linked by the phenomenon of contact ageing, which implies the strengthening of a contact with time and is usually related to an increase of contact area in the frame of multi-asperity models.

It is less clear, how contact ageing affects nanoscale systems of constant contact area. Recently, it was shown, that such systems (i.e. Sb nanoparticles sliding on HOPG) also experience contact ageing and that sliding can be described as a thermally activated process of contact strengthening and breaking [1].

New experiments with improved data acquisition have now revealed, that particle movement follows an irregular stick slip pattern, where the stick time can directly be interpreted as the 'age' of the contact and a logarithmic increase of contact strength with time is found. At the same time the ageing law also describes conventional static friction measurements, where the nanoparticle was fully resting. Effectively, this means that a universal ageing law can be applied over 6 orders of magnitude in time to describe likewise both static and sliding friction [2].

MD simulations for nanoparticles [3] suggest, that the observed ageing process is related to the formation of commensurate patches at the otherwise incommensurate interface.

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Submitted for a poster or a talk (talk preferred)

Role of surface roughness and viscoelasticity on rubber adhesion in dry and liquid environments

Adhesion between glass or acrylic balls and various types of rubber is investigated experimentally and analysed theoretically. The work of adhesion during pull-off varies strongly depending on the system studied, which we attribute to two opposite acting effects, namely viscoelastic energy dissipation close to the opening crack tip, and surface roughness. For soft silicone rubber compounds an additional process result in a strong increase in the work of adhesion with increasing pull-off velocity, which may result from non-adiabatic processes associated with chain pull-out.

We have distinguished the three major contributions to rubber adhesion acting at different length scales: bulk viscoelasticity, roughness and molecular mobility. The time-dependent viscoelastic contribution leads to higher adhesion for the softer compounds at the same velocities. The roughness contribution can have different sign depending on the stiffness of the rubber compound. This different behaviour can be explained by the additional elastic energy stored while contact formation of the stiffer rubber with the rough surface and the additional contact area in the case of the compliant softer rubber. Mobile molecules in the weakly cross-linked structures can get attached to the countersurface and are pulled out from the substrate accompanied with energy dissipation and the increased work of adhesion.

Gold on graphene and viceversa: prototypical nanoscale contacts with complex tribological response

R. Guerra, A. Benassi, L. Gigli, E. Tentori, A. Vanossi, N. Manini, E. Tosatti

The interface of gold with graphene (or graphite) constitutes a workhorse system for nanotribology, due to the possibility to achieve clean and well characterized contacts, hence favoring a crosscheck between simulations and experiments. Despite the weak -- mostly vdW -- Au/graphene interaction, responsible for the observed structural lubricity, the apparent simplicity of this interface is complicated by an interplay of geometric and energetics effects, which render the frictional response highly system-dependent. Here we consider two cases, gold nanocluster on graphite [1,2] and graphene nanoribbons on gold [3]. For each case I report, beside energetics considerations, the static and dynamic friction response classically simulated using state-of-the-art force-fields and methodology.

By means of these examples we show how size, shape, and dimensionality of the contact, can determine a variety of frictional regimes, and how the latter should behave when approaching the thermodynamic, macroscopic, limit.

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First principles investigation of frictional properties of graphene and 2D transition metal dichalcogenides

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In recent years, nanotribological properties of two dimensional (2D) materials, especially graphene and 2D transition metal dichalcogenides, has been subject to numerous studies. There are several calculations on these systems using molecular dynamics methods, but *ab initio* investigations are very limited because of large system sizes. In this work, we have investigated the sliding mechanisms and the frictional force between various graphene surfaces as well as transition-metal dichalcogenides (TMDCs) ones by performing quantum mechanical first-principles calculations, including dispersive van der Waals interactions as well, based on density functional theory. Friction properties of those homo- and hetero-flakes and bilayers of graphene and TMDCs are studied by performing friction force calculation under different load and environment (like defects, ad-atoms etc.) conditions. We determine the friction coefficients under low loads and analyze the variations in the electronic structure during slidingof the surfaces with respect each other. Based on these results, we provide an understanding of tuning the friction of these 2D materials at nanoscale. This work is supported by TUBITAK Project No: 114F162.

Is Partial Slip under Transverse Oscillatory Loading a Transient Event?

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Contacts subjected to reciprocating tangential loads often experience partial slip, also termed “microslip”. As all interfacial friction processes, partial slip introduces a *nonlinear* dependence of force on displacement. Such nonlinearities can be probed with acoustic resonators.

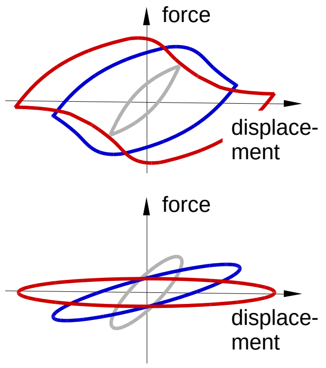

Fig. 1: Two different realizations of a transition from stick to gross slip in oscillatory motion. The force-displacement loop at the top follows from the Cattaneo-Mindlin model. The transition amounts to an instability. As sketched in the lower panel, the contact may also be in a predominantly linear state at all amplitudes, where contact stiffness and the dissipation varies with amplitude.

In previous work, we have used the amplitude dependence of the shifts in resonance frequency and bandwidth (Δf and $\Delta\Gamma$) of a quartz crystal microbalance (QCM) to study partial slip. If partial slip is present, an increase in oscillation amplitude leads to a decrease in frequency and an increase in bandwidth. One may view these shifts as indicative of a softening of the contact, meaning that the time-averaged contact stiffness decreases, while the time-averaged dissipation increases.[1]

This finding leaves open, whether the underlying friction loops are indeed nonlinear – as predicted by the Cattaneo-Mindlin model (top in Fig. 1). They might also remain ellipsoidal in shape, but become closer to horizontal (decreasing contact stiffness in the linear sense) and wider (increasing dissipation in the linear sense) as the amplitude increases. The second situation is expected when a state with partial slip does not return to stick at the turning points of the oscillation, but rather constitutes a stationary condition which allows for sliding. In the first case, the width of the sliding region, w, returns to zero at each turning point of the oscillation and grows as the displacement increases. In the second case, w remains constant over the entire cycle and evolves much slower than the period of oscillation. These two scenarios are limiting cases. The width of the sliding annulus may be some other function of time.

In principle, the dynamics of the nonlinearities can be addressed with third harmonic generation (THG).[2] Third harmonic generation in the context of the QCM at this point suffers from a lack of knowledge of the resonators (linear) response function at 3ω. This information is needed for quantitative analysis. Also, the 3ω-signal is not resonantly enhanced, which lowers its magnitude.

Making use intermodulation products[3] *we have undertaken intermediates step towards a full analysis of friction loop and its evolution with time.* In intermodulation analysis, the resonator is driven by two narrowly spaced sine-waves (at frequencies $\omega_0 \pm \Delta\omega$), the superposition of which produces a fast sinusoidal amplitude beat. From the response at the frequencies $\omega_0 \pm n\Delta\omega$ with n = 3, 5, 7, 9 ,11, … one can reconstruct the amplitude dependence of frequency and bandwidth. This is done with variable $\Delta\omega$, variable drive levels and varied states of the sample.

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NONLINEAR STOCHASTIC MODEL OF STICK-SLIP FRICTION DUE TO ICE SURFACE SOFTENING

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The ice surface softening during friction is shown as a result of the spontaneous appearance of shear strain caused by external supercritical heating. This transformation is described by the Kelvin-Voigt equation for viscoelastic medium, the relaxation equations of Landau-Khalatnikov-type and for heat conductivity. The study reveals that the above-named equations formally coincide with the synergetic Lorenz system, where the order parameter is reduced to shear strain, stress acts as the conjugate field, and temperature plays the role of the control parameter. The examination of dependence of the relaxed shear modulus on strain explains the ice surface premelting according to the first-order transition mechanism. The critical heating rate is proportional to the relaxed value of the ice shear modulus and inversely proportional to its typical value.

We examine the additive non-correlated fluctuations of the shear strain and stress, and the temperature. Taking into account the noises in the suggested basic equations the Langevin and Fokker-Planck equations are derived. Their analysis is based on investigation of extrema of the distribution function, i.e., steady state values of the shear strain, using the Stratonovich interpretation. The phase diagrams are constructed where noises intensities and thermostat temperature determine the existence regions of ice, softened ice, and their mixture (stick-slip rubbing). We present that domain of ice friction is bounded by relatively small background sliding block temperatures and fluctuations intensities of the stress and temperature. The ice film softens with growth of the stress noise intensity even at small thermostat temperatures. The friction force time series for all rubbing modes are calculated and compared with experimentally observed ones.

Giant dissipation peaks onto $SrTiO_3$ surface measured by pendulum AFM

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Bodies in relative motion separated by few nanometer gap experiences a tiny friction force, whose nature is not understood. This non-contact form of friction can be successfully measured by highly sensitive cantilever oscillating like a tiny pendulum over the surface [1].

Recently it was reported that the critical fluctuations at the phase transition in a bulk $SrTiO_3$ may affect the dissipation of mechanical probes even if completely external to the crystal surface [2]. Here, we report on striking multiplet of dissipation peaks above $SrTiO_3$ surface present at low temperatures (T=5K) and after sample annealing to high temperatures (T~1000°C) which leads to oxygen deficient sample. This is confirmed by change of electronic structure in the proximity of the Fermi energy as compared to moderate annealed sample. We believe that observed dissipation peaks are due to a change of valency/spin of the oxygen vacancy, or groups of vacancies, caused by the oscillating tip potential. Moreover the results show extremely strong dependence of dissipation peaks on external magnetic field.

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Sliding Friction of Graphene/*h*-BN Heterojunctions: Towards Robust Superlubricity

D. Mandelli, I. Leven, O. Hod, M. Urbakh

The miniaturization of mechanical devices calls for novel solutions to reduce frictional dissipation in regimes where standard lubrication approaches fail. Particularly promising for applications in nano- and micro-motive components are the lubrication properties displayed by rigid layered materials. Among the latter, graphene and hexagonal boron-nitride (*h*-BN) stand out for their extraordinary mechanical properties, which can provide the required interface robustness and durability. Furthermore, their intrinsic intra-layer lattice mismatch foreshadows the possibility to realize superlubric heterojunctions made thereof. To achieve microscopic understanding of the underlying tribological processes we perform fully atomistic molecular dynamics simulations of the sliding friction at graphene/*h*-BN interfaces. For the aligned, nearly-commensurate junctions we find a characteristic contact size above which superlubricity sets in due to the progressive appearance of the Moiré pattern. Breaking of superlubricity due to possible self-reorientation processes as observed in graphitic contacts is therefore avoided in large enough heterogeneous junctions. Incommensurability effects are enhanced in misaligned flakes, and kinetic friction is found to further reduce by 2-3 orders of magnitude. Our simulations also show that the superlubric regime persists up to significantly higher loads compared to the well-studied twisted homogeneous interface. This indicates the potential for achieving robust superlubricity in practical applications using 2D layered heterojunctions.

Bridging the gap between macro and nano-scale wear behavior: an experimental attempt.

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The development of the Atomic Force Microscopy (AFM) allows investigating wear at the nanometer scale. However, the wear rate is a slow process at the nano-scale, which renders fastidious quantitative measurements of the wear volume for determining wear laws. In this talk, we describe a new effective experimental methodology based on the Atomic Force Microscope Circular mode. Using this methodology, macroscale wear behaviour expressed through well-known Archard's and Barwell's law was compared with nanoscale wear behaviour of copper-based nanocomposite with Al_2O_3 nanoparticles.

Acknowledgement

These investigations were performed within the bilateral project between the Republic of Serbia and the French Republic, programme Pavle Savić – Partenariats Hubert Curien No. 451-03-39/2016/09/11 – 36239VA and COST Action MP1303. Aleksandar Vencl also acknowledges the project TR 35021, supported by the Republic of Serbia, Ministry of Education, Science and Technological Development, whose financial help is gratefully acknowledged.

(temporary abstract)

NANOFRICTION IN ROTATING COLLOIDAL RINGS

We investigate the nanofriction in two- or more circularly sliding adjacent colloidal rings. Each ring contains a different number of colloidal particles, intrinsically providing an incommensurate system. Upon a variation of the ring radii as well as the particle numbers in each ring, we are able to modify the incommensurability, and to reveal the frictional behaviour at various conditions.

Ballistic thermophoresis on graphene

Emanuele Panizon, Roberto Guerra, Erio Tosatti

If the temperature of a fluid is not uniform in space, a floating body may feel a thermophoretic force which is proportional to the local temperature gradient; the same relation could be assumed to hold for a nanometer sized object physisorbed on a 2D layer subject to an heat flow.

We employ Non-Equilibrium Molecular Dynamics (NEMD) to study a test system: a gold nanocluster adsorbed on free-standing graphene clamped between two temperatures ΔT apart. We find a phoretic force which for relatively large submicron lengths is parallel to, but roughly independent of, the gradient magnitude.

This signals a nonconventional thermophoresis that is ballistic in character. Subsequent analysis shows that the phoretic force is dominated by flexural phonons, whose flow is indeed known to be ballistic and distance-independent up to the relatively long scattering lengths that precede the standard diffusive regime.

Interestingly, ordinary harmonic phonons only carry pseudomomentum and could not exert a net force on a adsorbed object. Yet, the monolayer supports a specific anharmonic coupling between corrugation and 2D density which endow the flexural phonons with some real momentum, part of which is transmitted to the adsorbate through scattering. The resulting distance-independent thermophoretic force is not unlikely to possess practical applications.

Single Molecule Experiments to Explore Friction and Adhesion

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Controlled manipulation processes of single-molecules with an atomic force microscope (AFM) provide valuable information about their interactions with surfaces, leading to fundamental insights into adhesion and friction properties. To understand such phenomena at the molecular level, tuning-fork based AFM operated at low temperature and in ultra-high vacuum is an appropriate tool since complex manipulations of a single molecule are possible [1]. With such approach however, the measured frequency shifts are related to normal force gradients, and thus the interpretation of friction phenomena is not fully straightforward. To overcome this issue, we combined original experiments with appropriate analytical models in order to determine adhesive energy and nanoscale friction of those single molecules at surfaces. In this presentation, few examples of single-molecule manipulation experiments [2] will be presented consisting in either their vertical pulling or lateral dragging of various organic adsorbates such as polymeric chains, graphene nanoribbons or single porphyrins. The forces gradient variations experimentally observed that way were found to be related to the interplay between intra-molecular mechanics, adhesion and friction properties and is supported by the analytical models as well as numerical calculations. These results pave the way to the field of "single-molecule tribology".

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Describing electronic friction: electron wind in a toy model

Davide Mandelli, Franco Pellegrini, Erio Tosatti

The electronic contribution to friction, often neglected in mesoscopic descriptions, can become quite relevant in the realm of nanofriction. While at macroscopic level electric resistance is trivially due to electronic scattering and Joule effect to the resulting dissipation, these effects are rarely described at microscopic level in the context of friction.

We propose an approach where we simulate the coupled electrons and ions dynamics in a simple toy model by projecting the electronic wavefunction on a time dependent basis of atomic orbitals. The electromotive force is included via a time dependent vector potential exploiting periodic boundary conditions in our model.

We are able to reproduce a qualitatively realistic microscopic picture of current, resistance and its counterpart as momentum transfer to the system. Introduction of an adatom results in what is commonly referred to as "electron wind", relevant to the description of electromigration. Application to more complex systems could provide a coherent picture of electronic friction with theoretical and technological relevance.

Manipulation of organic molecules (ssDNA and pyrene chains) over a gold surface: insights from atomistic MD simulations.

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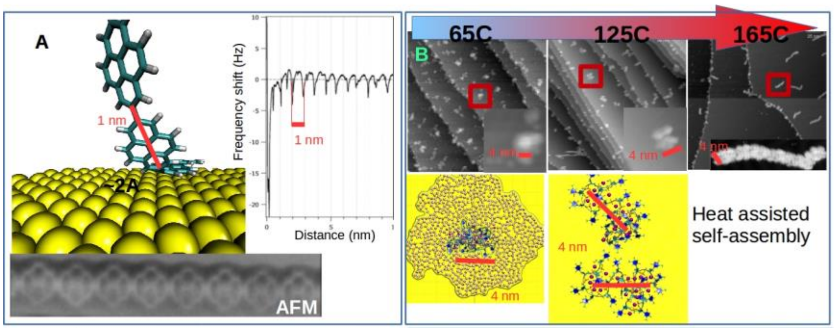
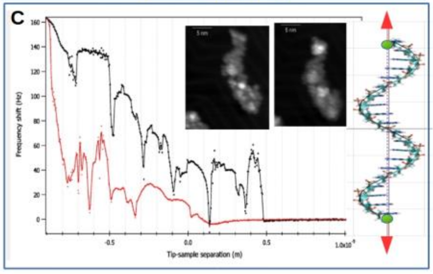
The design of molecular machines capable of directional motion on a surface constitutes nowadays an active field of scientific research[1,2,3]. In order to control/optimize these molecular machines, it is of paramount importance to know how friction operates at a molecular level. Recent advances in scanning probe techniques allow us to not only characterize with very high resolution molecules over surfaces, but also they have opened the possibility to obtain a thorough description of their mechanical properties[3,4,5].

In this work, we consider two very distinct molecules so to address how their internal complexity affects the overall mechanical response. In particular we study ssDNA- single-stranded-DNA (20-mer-cytosine) and a simpler chain, i.e. a 20-mer-pyrene over a Au111 surface. Here we use atomistic molecular dynamics simulations [6] to mimic the experimental conditions/processes, in particular: annealing, lifting off molecules from the surface and sliding them over the surface. For ssDNA molecules we show how the speed of annealing/quenching cycles allow us to control the size of the self-assembly, and, in some cases, so to achieve large and well-structured assembly of ssDNA molecules. Then for both molecules (ssDNA and pyrene) we perform MD simulations so to mimic the molecule-surface detachment process as in the experiments. Here we observed that while pyrenes experience a single unit base detachment at a time (in a stick-slip manner), for ssDNA molecules, this process is much more complex. While for pyrenes the dominant interaction was the one with the surface, for ssDNA molecules, the dominant interaction was the one with itself. So the upward pulling process, although it also occurs in a stick-slip manner with the length of the slip corresponding to the nucleotide base distance, the corresponding force curve is much more richer and entails many more details about the molecule itself than in the pyrene case. At last, we also simulated the sliding of a single pyrene chain over a Au(111) surface. As in the experiments we found that the friction depends on how many units we detach from the surface. Here our MD simulations provide a thorough description of the overall process relating the change in the friction contrast with the number of detached units to the fact that the torsional stiffness of the molecule is changing as one desorbs it from the surface.





Caption:
A) Lifting off pyrene from a gold111 surface. MD simulation snapshot, CO-AFM tip image and frequency shift as measured in the experiments
B) Process of heat assisted self-assembly of ssDNA over gold111. Top row experimental STM images, bottom row MD simulation results
C) Lifting off ssDNA assembly from surface. MD results show the forces measured correspond to the DNA unfolding over gold111 surface.

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Wide dynamic range 2-D nanoindentation: Initiation of slip and effects of initial plasticity

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A new nanomechanical testing system is described. It provides the same force controlled displacement sensing capability as nanoindentation, but now with two completely separated orthogonal axes. Load modulation enables direct determination of contact area and stiffness, both lateral and vertical, along with energy losses from the phase shifts. Two features in particular, wide dynamic ranges of several orders of magnitude of stiffness, and a very high degree of mechanical separation (low crosstalk) between the axes, distinguish the technique from AFM. As a result, the evolution of a contact under 2-D stresses from deformation-free atomistic scale to initial plasticity with its associated changes in geometry, can be monitored. Results will be presented showing that Mindlin partial slip does not occur immediately under lateral stress in slightly plastically deformed contacts. The evolution of contact area in the initial stages of sliding in the presence of plastic flow will also be described, and resembles the predictions of classical Tabor and Johnson models.

Ab Initio Study of Frictional Properties of Graphene over 4H-SiC{0001} Surfaces

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We investigated the frictional properties of graphene deposited onto a silicon carbide substrate throught a first principles study. Surface energy profiles are obtained by sliding the top-most layer of bi-, tri-, tetra- and pentalayer graphene systems stacked on both the Si- and C-terminated faces of 4H-SiC{0001}. The first graphene layer forms a stationary corrugated buffer layer covalently bonded to the surface at the interface and the energy profiles reveal that the static friction of additional graphene sheets depends upon layer thickness as well as the properties of the underlying SiC substrate. Our results are further discussed by examining the changes in the band structures and extracting the charge density differences along sliding pathways. This work is supported by TUBITAK Project No:114F162.

Limitations of structural superlubricity: Chemical bonds versus contact size

Dirk Dietzel, Ján Brndiar, Ivan Štich, and André Schirmeisen

Structural superlubricity describes the state of virtually frictionless sliding if two atomically flat interfaces are incommensurate, i.e. they share no common periodicity. Despite the exciting prospects of this low friction phenomenon, there are physical limitations to the existence of this state. Theory predicts that the contact size is one fundamental limit, where the critical size threshold mainly depends on the interplay between lateral contact compliance and interface interaction energies. Here we provide experimental evidence for this size threshold by measuring the sliding friction force of differently sized Antimony particles on MoS_2. We find that superlubric sliding with the characteristic linear decrease of shear stress with contact size prevails for small particles with contact areas below 15,000 nm^2. Larger particles, however, show a transition towards constant shear stress behavior. In contrast, Sb particles on graphite show superlubricity over the whole size range. Ab initio simulations reveal that the chemical interaction energies for Sb/MoS_2 are much stronger than for Sb/HOPG and can therefore explain the different friction properties as well as the critical size thresholds. These limitations must be considered when designing low friction contacts based on structural superlubricity concepts.

For presentation at International Conference on Trends in Nanotribology, 26-30 June 2017, Trieste ITALY

Linking microstructure to wear-induced pitting corrosion in aged 2507 super duplex stainless steel

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Grade 2507 super duplex stainless steel ordinarily achieves a balance of corrosion resistance and mechanical properties through its dual phase ferrite-austenite microstructure. However, heat treatment in the 600-900°C temperature range causes phase transformations to occur, developing complex microstructures with secondary phases including sigma phase, secondary austenite, chi phase, and chromium nitrides. It has already been demonstrated that in tribocorrosion experiments in 0.6 M NaCl in anodic potentiostatic conditions, the passivity of aged 2507 is eliminated due to mechanical wear, and pitting can occur in and near the wear track. However, the precise mechanism of this loss of passivity is not yet understood. In the present study, we explore the tribocorrosion behavior at selected phases and grain boundaries. Correlating the microstructural features to local surface topography changes and the current transient response promises to reveal precise details of the wear-induced corrosion behavior.

Image states and energy dissipation on Bi$_2$Te$_3$ surface

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Topological insulators (TIs), belonging into the family of intercalated compounds, have a bandgap in the bulk that makes the crystal insulator, whereas their surfaces (or edges) are conducting. While protected topological states might offer promising playground to observe exotic physical phenomena like Majorana fermion bounded state [1] or magnetic monopoles [2], the effect of friction on topologically proteced surface is yet to be reported.

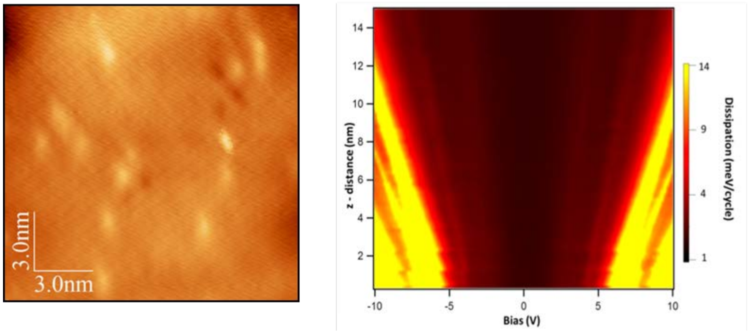

Fig. 1: (left) STM image of Bi$_2$Te$_3$ crystal at 5K. Surface of native Bi$_2$Te$_3$ is characterized by large defects density. Tunneling parameters: I_t= 300pA, V_b= 330 mV. (right) Energy dissipation map plotted versus distance and tip-sample voltage (on defect free Bi2Te3). Bright contrast represents high dissipation. Series of dissipation spikes are visible on the map.

Here we study energy dissipation onto Bi$_2$Te$_3$ surface by means of pendulum geometry oscillating cantilever of combined AFM/STM [3]. While STM shows well understood image potential states, AFM reports on huge dissipation peaks occur due to charging/discharging of those states by the oscillating tip. Huge dissipation peaks occur few nm above the surface and are localized at relatively large voltages as expected for image states. Moreover the energy dissipation depends on the local defect density.In order to understand the frictional response of Bi$_2$Te$_3$ in TI phase as well as its frictional response when the TI phase is partially or fully suppressed, we probe surfaces with different defect density and under external magnetic field. The results show extremely strong dependence of dissipation on external magnetic field since the peaks are shifted to lower energies as the magnetic field increases.

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The use of nanoparticles in the enhancement of the tribological properties of conventional lubricating oils

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Superior tribological properties of nanolubricants have been recently well established for conventional oils, and enhancing the tribological performance of lubricants with nanoparticle additives is currently an active area of research. Recently scientists used nanoparticles in different tribological systems and nanolubricants have been widely studied as an alternative solution to conventional lubricant oils, since they allow obtaining significant reduction of friction and improvements of load-carrying capability. The action of nanoadditives reduces friction and wear on surfaces that operate in sliding contact with each other. Of particular interest are graphene and carbon based nanomaterials, such as Carbon Nanohorns (CNHs) and Carbon Nanotubes (CNTs). CNHs have been the subject of numerous studies due to their unique morphology and wide ranging properties of graphene, including chemical stability, low surface energy and high thermal and electrical conductivity. However, limited investigations were carried out on their tribological and anti-wear properties.

Herein, a summary about last studies carried out on different nanolubricant systems is presented. The enhancement of tribological properties of nanofluids containing CNHs is reported, that deals also with the differences in anti-friction and anti-wear capabilities of these systems, due to a variation of the surface topology of the substrate, in terms of roughness, and operating temperature. Nanofluids developed for different applications were selected, i.e. for refrigeration/air-conditioning sector and for automotive/cogeneration field.

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