O 109: Tribology and Structure of Surfaces: Misc.

Time: Friday 10:30–13:00 Location: WIL A317

Invited Talk O 109.1 Fri 10:30 WIL A317

Discovery of 1D spin-polarized states at step edges of topological crystalline insulators — •Paolo Sessi — Universität Würzburg

Topological crystalline insulators (TCIs) are topological materials where the existence of surface Dirac states is guaranteed by crystal symmetries. This protection mechanism promises a rich phenomenology in response to crystal perturbations. In my presentation, I will report on the discovery of robust 1D spin-polarized channels naturally emerging at TCI surfaces once translational invariance is broken [1]. I will illustrate how 1D channels can be easily obtained in the prototypical TCI $Pb_{1-x}Sn_xSe$ without the need of any sophisticated preparation technique. In particular, by correlating topographic and electronic structure information, I will show that 1D states naturally emerge at step edges consisting of an odd number of atomic layers, where translational invariance is broken, while even step edges maintain translational symmetry and are featureless. By systematically acting on the crystals stoichiometry, I will demonstrate how these 1D states are directly linked to the existence of a topologically non-trivial bulk band structure. A minimal toy model and realistic tight-binding calculations allow to identify them as spin-polarized at bands connecting two Dirac points. Finally, I will show how, contrary to 1D topological states known so far, their protection mechanisms result in a striking robustness to defects, strong magnetic fields, and elevated temperature.

[1] P. Sessi *et al.*, Science *in press.*

O 109.2 Fri 11:00 WIL A317

Temperature dependent Contact Ageing effects for Diamond and Silica Interfaces — •Matthias Vorholzer, Dirk Dietzel, and André Schirmeisen — Institute of Applied Physics, Justus-Liebig-University, Giessen, Germany

Contact ageing describes the temporal evolution of interface conditions. While this topic is well known on the macroscale, recent experiments have shown, that ageing can also play an important role in nanoscale contacts [1,2,3], where ageing is supposed to influence parameters like e.g. interface matching, contact area, or the apparent stiffness of a contact. In most cases nanoscale contact ageing is assumed to be a thermally activated process. Thus, temperature dependent measurements are a viable way to survey and thoroughly explore the relevant interface processes. Here, we present experimental data with well-defined ageing times up to 10 s for Silica-Silica and Silica-Diamond interfaces, gathered with an UHV-AFM between 15 K and 300 K using the slide-hold-slide protocol [1]. Our experimental approach gives access to both static friction and contact stiffness, which can then be compared to theoretical predictions. For each temperature the anticipated logarithmic ageing is observed, yet the temperature dependence contradicts simple scenarios based solely on thermal activation [2]. Thus, more complex and realistic ageing scenarios are currently considered to describe all aspects of contact ageing.

[1] Q. Li et al., Nature 480, 233 (2011)
[2] M. Feldmann et al., PRL 112, 155503 (2014)
[3] M. Feldmann et al., PRL 117, 025502 (2016)

O 109.3 Fri 11:15 WIL A317

Antimony Nanoparticles Sliding on MoS_2: The Breakdown of Superlubricity — •Dirk Dietzel[1], Jan Brndiar[2], Ivan Stich[2], and Andre Schirmeisen[1] — [1]Institute of Applied Physics, University of Giessen, Germany — [2]CCMS, Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia

Structural lubricity is an intriguingly simple concept, that predicts ultra-low friction between substrate and slider as long as a structural mismatch prevents effective interlocking of atomic potentials at the interface. In principle, this concept should be applicable to almost any material combination. However, in experiments it is found that superlubricity is rather exotic than widespread. Often, Interface contamination must be considered a limiting factor. But even under ideal conditions, structural superlubricity can be inhibited by the mechanical stability of the materials [1]. Here, we analyze this aspect by nanomanipulation experiments for Sb nanoparticles on HOPG and MoS_2. Despite the similarity of these layered lubrication materials, both show significantly different frictional behavior. More specifically, MoS_2 shows a breakdown of superlubricity, which becomes evident by checking the scaling laws of structural lubricity [2]. To explain this breakdown we have performed additional DFT simulations, which revealed significantly heightened interface interactions, that are sufficient to drive the Sb/MoS_2 system out of superlubricity.

[1] T .A. Sharp, L. Pastewka, M. O. Robbins. PRB 93, 121402 (2016)
[2] D. Dietzel, M. Feldmann, U. D. Schwarz, H. Fuchs, A. Schirmeisen. PRL 111, 235502 (2013)

O 109.4 Fri 11:30 WIL A317

Effect of additives and external fields on lubricating properties of nematic liquid crystals — •Pritam Kumar Jana[1], Wei Chen[2], Mikko J. Alava[1], and Lasse Laurson[1] — [1]COMP Centre of Excellence, Department of Applied physics, Aalto University, P.O. Box 11100, Aalto 00076, Finland — [2]Computer Network Information Center, Chinese Academy of Sciences, Beijing 100190, China

Several studies have been performed to understand the structural and dynamical properties of liquid crystal lubricants under external pressure and shear stress, mainly due to the observations of ultra-low friction in such systems [1]. However, to balance between efficiency and effective cost, more extensive investigations are required. In the present study, we construct a full atomistic model where a nematic liquid crystal, 4-cyano-4-hexylbiphenyl (6CB), and a short alkane chain, hexane (C6H14), are used as lubricant and additives, respectively, and mica serves as the confining surfaces. When the sliding velocity of the upper mica plate is low enough, thin films of both pure 6CB and pure C6H14 show stick-slip dynamics. However, for the same film thickness liquid crystals exhibit higher friction as compared to hexane. In addition for thick films effective viscosities of pure liquid crystals remain constant and approximately similar to bulk viscosity. When film thickness decreases effective viscosities increase. We also consider mixtures of 6CB and C6H14, by varying their proportions, as well as the effect of external electric fields, to study the resulting lubrication properties.

[1] C. Manzato, A. S. Foster, M. J. Alava, and L. Laurson. Physical Review E 91, 012504 (2015)

O 109.5 Fri 11:45 WIL A317

Temperature dependent investigation of Ni layers on Pd with Positron annihilation induced Auger electron spectroscopy, XPS and STM — •Samantha Zimnik, Marcel Dickmann, Sebastian Vohburger, and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ) and Physik Department E21, Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany

Positron annihilation induced Auger Electron Spectroscopy (PAES) is a powerful technique to gather information about the elemental composition of the topmost atomic layer of a specimen. The positron beam facility NEPOMUC at the research reactor of the Heinz Maier-Leibnitz Zentrum in Garching delivers the world's most intense positron beam and enables measurement times of only a few minutes per PAES spectrum. A new sample holder allows controlling of the sample temperature during the measurement up to 500°C. Thus, time and temperature-dependent PAES have become possible and hence enable the in-situ observation of the surface segregation process. The surface spectrometer at NEPOMUC uses the complementary techniques PAES, X-ray photoelectron spectroscopy (XPS) and Scanning Tunneling Microscopy (STM) to characterize both, the elemental composition of the surface and its topology. Recent studies on sub-monolayers of Ni on Pd using time- and temperature dependent PAES will be presented.

O 109.6 Fri 12:00 WIL A317

Dipole-mediated single-molecule manipulation — •Grant Simpson[1], Víctor García-López[2], James Tour[2], and Leonhard Grill[1] — [1]University of Graz, Graz, Austria — [2]Rice University, Houston, Texas, USA

It has been long known that the scanning tunneling microscope (STM) is the perfect tool not only for imaging single molecules on surfaces, but also can be used to manipulate such molecules in a variety of ways. The classical method of lateral manipulation is either pushing or pulling via van der Waals interaction with the STM tip. In the current work it is shown that the electric field of the tip plays an important role when a dipole moment exists within a molecule. The dipolar

nanocar, investigated here on the Ag(111) surface, displays rotational and translational motion under the influence of the electric field of the tip. Furthermore, the spatial dependence of the tip position with respect to the molecule reveals that the dipole moment of the molecule is the deciding factor for the direction of motion. The rotation and translation of the nanocar can therefore be carefully controlled.

O 109.7 Fri 12:15 WIL A317

Tiefenaufgelöste Wasserstoffinventarbestimmung mittels Massenspektroskopie nach Laserablation — •Jannis Oelmann, Niels Gierse, Sebastijan Brezinsek, Michaele Freisinger und Christian Linsmeier — Institut für Energie und Klimaforschung - Plasmaphysik, Forschungszentrum Jülich GmbH, 52425 Jülich, Deutschland

Eine quantitative Bestimmung des Wasserstoffgehalts in Materialien wie Metallen oder funktionellen Schichten ist essentiell in Herstellungsprozessen, beispielsweise von Solarzellen oder Festkörperbatterien. Vorgestellt wird eine Methode zur tiefenaufgelösten Bestimmung des absoluten Wasserstoffgehalts von Festkörpern ohne Probenpräparation. Zur besseren Unterscheidung vom Hintergrund wird das Wasserstoffisotop Deuterium (D_2) in Titandideuteridschichten auf Wolframsubstraten, welche mittels Magnetronsputtern hergestellt wurden, detektiert. Der Partialdruck von Deuterium wird dazu in einer Vakuumkammer nach Einzelschuss-Laserablation über Quadrupolmassenspektroskopie bestimmt. Eine quantitative Bestimmung des Deuteriumgehalts der Probe wird durch Kalibration des Massenspektrometers über Kalibrationslecks ermöglicht. Es wird die dritte Harmonische ($\lambda = 355$ nm) eines Nd:YVO_4-Lasers mit einer Impulsenergie von bis zu $E = 50$ mJ bei einer Laserimpulslänge von $\tau = 35$ ps genutzt. Folglich liegt für diese Laserparmeter die thermische Eindringtiefe in der gleichen Größenordnung wie die optischen Eindringtiefe, was schussaufgelöste Tiefenprofilmessungen durch weitere Ablationsprozesse an der selben Probenposition ermöglicht.

O 109.8 Fri 12:30 WIL A317

Chemistry of artificial 2D orbitals — •Aizhan Sabitova[1,2], Jeffrey Rawson[2,3,4], Stefan Tautz[1,2], and Ruslan Temirov[1,2] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, Germany — [2]JARA - Fundamentals of Future Information Technology — [3]Peter Grünberg Institute (PGI-6), Forschungszentrum Jülich, Germany — [4]Institute of Inorganic Chemistry, RWTH Aachen, Germany

Two-dimensional (2D) electron systems represent a fascinating area of research. Several bottom-top approaches to engineering of such systems with defined energy spectra have been presented recently [1-4]. In our work we pattern a commensurate monolayer of 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) on Ag(111) using a low-temperature scanning tunneling microscope to produce vacancies and study their electronic structure. Produced vacancies possess electronic orbitals that appear as a bound state below the onset of dispersive 2D interface state of PTCDA/Ag(111). Orbitals of two vacancies interact to form bonding and anti-bonding pair of orbitals, shapes of which were visualized by scanning tunneling spectroscopy imaging. This hybridization can be readily understood by analogy with chemically interacting s-orbitals. We show that vacancy structures of more complex shapes demonstrate effects of multi-orbital hybridization.

[1] K.K. Gomes et al., Nature 483, 306-310 (2012) [2] K. Seufert et al., Nano Lett. 13, 6130-6135 (2013) [3] W-X. Qiu et al., arXiv:1609.01876v1 [4] R. Drost et al., arXiv:1611.01049v2

O 109.9 Fri 12:45 WIL A317

Monitoring corrosion in nano confinement in real time using white light interferometry — •Claudia Merola[1], Hsiu-Wei Cheng[1], Ying-Ju Chen[1], and Markus Valtiner[2] — [1]Max Planck Institute, Düsseldorf, Germany — [2]Technische Universität Bergakademie, Freiberg, Germany

Crevice corrosion (CC) still remains one of the most difficult types of corrosion to detect and to prevent. Most often CC occurs in narrow fissures where oxygen access is poor and a stagnant electrolyte solution is present. Experimentally it is a challenge to obtain in-situ information of processes in confined geometries and to establish well defined confined situations in the first place. Here, white light interferometry has been used, for the first time, to study and monitor in situ the initial stages of the crevice corrosion process of thin layers of Nickel in different concentrations of NaCl solutions. Using Mica as a crevice former in an electrochemical surface apparatus allowed us to provide a deeper understanding of the initiation of the corrosion process. Electrochemical potential ramps were applied at different rates and different concentrations of NaCl led to different corrosion mechanism, based on a variation of the material transport mechanism into and out of the confined zones. Our results reveal that CC proceeds as a self-catalyzed pitting inside the confined zone and provides a surprising real-time view of the initial corrosion of confined surfaces, and hence may contribute to a deeper general understanding, and ultimately prevention, of localized corrosion.