O 84: Nanotribology

Time: Thursday 16:00–17:30 Location: WIL B321

O 84.1 Thu 16:00 WIL B321

Theory of charge-density-wave noncontact phase slip nanofriction — •Franco Pellegrini[1,2], Giuseppe E. Santoro[1,2,3], and Erio Tosatti[1,2,3] — [1]SISSA, Via Bonomea 265, I-34136 Trieste, Italy — [2]CNR-IOM Democritos National Simulation Center, Via Bonomea 265, I-34136 Trieste, Italy — [3]nternational Centre for Theoretical Physics (ICTP), P.O. Box 586, I-34014 Trieste, Italy

Bulk dissipation caused by charge-density-wave (CDW) voltage-induced depinning and sliding is a classic subject. We present a local, nanoscale mechanism describing the occurrence of distance-dependent dissipation in the dynamics of an atomic force microscope tip oscillating over the surface of a CDW material. A mechanical tip hysteresis is predicted in correspondence to localized 2π slips of the CDW phase, giving rise to large tip dissipation peaks at selected distances. Results of static and dynamic numerical simulations of the tip-surface interaction are believed to be relevant to recent experiments on the layered compound $NbSe_2$.

O 84.2 Thu 16:15 WIL B321

Self-Assembled Monolayers under Mechanical Stress — Christian Meltzer, Jonas Paul, Wolfgang Peukert, and •Björn Braunschweig — University of Erlangen-Nuremberg; Institute of Particle Technology (LFG), Cauerstrasse 4, 91058 Erlangen

The molecular structure of mechanically compressed octadecylphosphonic acid self-assembled monolayers (ODPA SAMs) on α-Al_2O_3 is studied with co-localized vibrational sum-frequency generation (SFG). The excellent stability of our custom-built manipulation device and SFG spectrometer has allowed us to apply defined normal forces and to probe the contact area in-situ with SFG over hours without significant drift which has also facilitated time resolved studies of compressed SAMs. Normal pressures up to 208 MPa are applied and load dependent SFG spectra are recorded as a function of pressure and lateral position relative to the center of contact. These co-localized SFG spectra allow for a comparison of measured contact areas with theoretical predictions from Hertzian theory. A detailed analysis of vibrational SFG spectra shows that both intensity and relative contributions of methylene and methyl vibrational bands to the SFG intensity are excellent indicators for pressure dependent changes in the molecular structure of ODPA SAMs. Analysis of SFG spectra provides strong evidence for the formation of gauche defects. In fact, after load release healing of defects occurs on two different time scales - a fast recovery and a slow process over a time period of several hours. The former is indicative for healing of shallow defects close to the head group while the latter is dominated by high energy barrier defects close to the anchor group.

O 84.3 Thu 16:30 WIL B321

Ab-initio modelling of energy dissipation in nanotribological systems. A DFT study of fcc Cu(111). — •Michael Wolloch[1,2], Gregor Feldbauer[1,2], Josef Redinger[1], Peter Mohn[1], and András Vernes[1,2] — [1]Institute of Applied Physics, Vienna University of Technology, Gußhausstraße 25-25a, 1040 Vienna, Austria — [2]Austrian Center of Competence for Tribology, Viktor-Kaplan-Straße 2, 2700 Wiener Neustadt, Austria

Accurate modelling of the energy dissipation in sliding friction with *ab-initio* methods in nanotribological systems poses a fundamental challenge in modern tribology. Here we present a quasi-static model to obtain the nanofrictional response of dry, wearless systems based on quantum mechanical all electron calculations. We propose a mechanism for energy dissipation, which relies on the atomic relaxations during sliding. Since our approach does not impose any limits on lengths and directions of the sliding paths, we investigate two different ways of calculating the mean nanofriction force, both leading to an exponential friction versus load behaviour for all sliding directions. We investigate arbitrary sliding directions for an fcc Cu(111) interface and detect two periodic paths which form the upper and lower bound of nanofriction. For long aperiodic paths the friction force convergences to a value in between these limits. For low loads we retrieve the Derjaguin generalization of Amontons-Coulomb kinetic friction law which appears to be valid all the way down to the nanoscale. We observe a non-vanishing Derjaguin-offset even for atomically flat surfaces in dry contact.

O 84.4 Thu 16:45 WIL B321

Plasticity during Contact of Rough Solids — •Tristan A. Sharp[1], Lars Pastewka[2], and Mark O. Robbins[1] — [1]Johns Hopkins University, Baltimore, USA — [2]Fraunhofer-IWM, Freiburg, Deutschland

Surfaces of many solids exhibit multiscale roughness which has important consequences for contact area, contact stiffness, and friction. Continuum theories and simulations typically can not treat certain atomic-level features despite indications of their importance. For example, the atomic steps on the surface of crystalline solids can alter the contacting area predicted by continuum. Similarly, an appropriate model of yielding is necessary to capture the spatial distribution of surface pressure in the contact. Here, we use large-scale molecular dynamics simulation to study elastoplastic contact between self-affine rough solids. We observe that the elastic continuum result of linearity between contact area and load at small loads is preserved, but with a larger proportionality constant due to yielding. The spatial distribution of contact area is modified only at short length scales. Atomic steps concentrate the stress, increasing the amount of plasticity and contact area. The mean pressure of contacting regions is then given as a decreasing function of atomic step density.

O 84.5 Thu 17:00 WIL B321

Scaling laws of friction: Area, time and temperature — •Dirk Dietzel, Michael Feldmann, and Andrè Schirmeisen — Institute of Applied Physics, Justus Liebig University Giessen, Germany

The investigation of friction by AFM assisted nanoparticle manipulation has presented itself as a very useful approach to gain insight into tribological processes of extended nano- and mesocontacts. Currently, this approach is utilized to analyze the significance of dynamic processes at the interface formed between particles and substrates. Our studies reveal that some experiments, like the contact area dependence of friction, can be explained by purely structural considerations of rigid interfaces, whereas other experiments, like the combined velocity and temperature dependence of interfacial friction, highlight the importance of dynamic interface processes, i.e. contact ageing and thermal activation. Comparing these experiments thus sheds a light on the validity of assuming rigid interfaces, with possible ramifications on the concept of structural lubricity. Additionally, we will show how measuring stick slip during nanoparticle sliding can be viable route to further analyze interface processes.

O 84.6 Thu 17:15 WIL B321

Adhesion and material transfer between contacting Al and TiN surfaces from first principles — •Gregor Feldbauer[1,2], Michael Wolloch[1,2], Peter Mohn[1], Josef Redinger[1], and Andras Vernes[1,2] — [1]Vienna University of Technology, Gusshausstrasse 25-25a/134, 1040 Vienna, Austria — [2]Austrian Center of Competence for Tribology, 2700 Wiener Neustadt, Austria

Contacts of surfaces at the atomic length scale are of fundamental interest for a better understanding of nanotribological processes, which are crucial in modern applications from nanoindentation or AFM/FFM to nanotechnologies applied in NEMS/MEMS.

A series of density functional theory (DFT) simulations was performed to investigate the approaching, contact and subsequent separation of two atomically flat surfaces consisting of various materials. Here, aluminum (Al) and titanium-nitride (TiN) slabs were chosen as a model system representing the interaction between soft and hard materials. The approaching and separation were simulated by moving one slab in discrete steps and allowing for electronic and ionic relaxations after each step. Various configurations of the interface were analyzed by considering (001), (011) and (111) surface orientations as well as several alignments of surfaces. The performed simulations revealed the influences of these aspects on the adhesion, equilibrium distance, charge distribution and material transfer. Material transfer in particular was observed for configurations where the interface is stronger than the softer material in the system, in the sense that the adhesion energy was found larger than the energy cost to remove surface atoms.