O 39: Tribology

Time: Wednesday 10:30–12:15 Location: H6

O 39.1 Wed 10:30 H6

Automated calculation of surface energies of arbitrary crystals — •Firat Yalcin and Michael Wolloch — Computational Materials Physics, Faculty of Physics, University of Vienna, Kolingasse 14-16, 1090 Vienna

The surface energy is one of the most fundamental properties of the surface facets of a crystal, determining the stability, equilibrium shape, catalytic activity, and other phenomena like surface segregation and roughening. In this work, we present a high-throughput workflow to calculate the surface energies of arbitrary crystals, accounting for all possible Miller indices and different terminations, using density functional theory (DFT). By employing available open-source libraries and custom-made tools, every step from querying bulk structures from various databases to the generation of slabs with precise geometries and subsequent DFT calculations is performed automatically and with minimal user input. Surface energies, Wulff shapes, as well as all in- and outputs, are automatically saved into an easily accessible, OPTIMADE compliant database. Example results are presented for some non-trivial surfaces with complex geometries to showcase the capabilities and validate our approach.

O 39.2 Wed 10:45 H6

High-throughput calculations of heterogeneous interfaces for tribology — •Michael Wolloch[1,2], Gabriele Losi[3], Omar Chehaimi[3], Firat Yalcin[1], Mauro Ferrario[4], and M. Clelia Righi[3] — [1]CMP, University of Vienna, Vienna, Austria — [2]VASP software GmbH, Vienna, Austria — [3]DIFA, University of Bologna, Bologna, Italy — [4]FIM, UNIMORE, Modena, Italy

We have shown in the past that fundamental properties of sliding interfaces like adhesion, friction, and ultimate strength, are closely connected to one another and the re-arrangement of charge at the interface [1-3]. We extended the previously presented approach for homogeneous interfaces to nearly arbitrary interfaces of crystalline surfaces, allowing us to treat heterogeneous interfaces of multi component systems [4].

In this talk we will present the fault tolerant and fully automatic workflow we developed, as well as initial results of the ongoing high-throughput studies we are conducting.

Part of this work was supported by ERC grant 865633 (SLIDE); [1] Wolloch et al. Sci. Rep. 9, 17062 (2019), [2] Restuccia et al. Comput. Mater. Sci., 154:517-529 (2018), [3] Wolloch et al. PRL 121, 026804 (2018) [4] Wolloch et al. Comput. Mater. Sci., 207:111302 (2022)

O 39.3 Wed 11:00 H6

The Influence of Temperature and Wear on Nanoscale Friction Anisotropy — •Jennifer Konrad, Dirk Dietzel, and Andre Schirmeisen — Institute of Applied Physics, Justus-Liebig University Giessen, 35392 Giessen, Germany

On atomically flat surfaces, the nanoscale friction force measured by atomic force microscopy shows a distinct variations dependent on the sliding direction of the AFM-tip. This anisotropy occurs as a consequence of the surface structure and is related to different energy barrier heights along different directions of the sample surface. In this work, this anisotropy of friction force is now analyzed as a function of temperature under UHV conditions on hexagonal latices like HOPG or MoS2 and also on ionic crystals with 90 degree symmetry like NaCl. At low sample temperatures, the friction force as deduced from the thermally activated Prandtl Tomlinson Model increases, and thermally activated random jumps become more unlikely, which direct influences the stability of the different sliding directions. This can be confirmed for HOPG and MoS2, while, our results for the ionic crystals additionally show that the both the absolute friction and the anisotropy are not only influenced by temperature, but also reflect temperature dependent wear effects.

O 39.4 Wed 11:15 H6

Dissipative frictional mechanism over Moiré superstructure — •Yiming Song[1], Xiang Gao[2], Antoine Hinaut[1], Sebastian Scherb[1], Shuyu Huang[1], Oded Hod[2], Michael Urbakh[2], and Ernst Meyer[1] — [1]Department of Physics, University of Basel, Basel, Switzerland — [2]Department of Physical Chemistry, School of Chemistry, The Raymond and Beverly Sackler Faculty of Exact Sciences and The Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv, Israel.

Friction force microscopy experiments performed on graphene-coated platinum surfaces that exhibit a variety of moiré superstructures demonstrate that, in addition to the well-known atomic stick-slip dynamics, a new dominant energy dissipation mechanism emerges. The observed velocity dependence of friction displays two distinct regimes: (i) at low velocities, the friction force is small and nearly constant; whereas (ii) above some threshold, friction increases logarithmically with velocity. The threshold velocity, separating the two frictional regimes, decreases with increasing normal load and moiré superstructure period. Atomistic molecular dynamics simulations demonstrate that the main contribution to frictional energy dissipation results from the elastic deformation and subsequent relaxation of moiré ridges caused by the pushing action of the tip as it slides over the superstructure. Based on the simulation results we develop a semi-phenomological model, which makes it possible to calculate friction under measurement conditions and provides excellent agreement with the experimental observations.

O 39.5 Wed 11:30 H6

Investigating thermal and directional motion in molecular friction processes by photonic force microscopy — •Subhrokoli Ghosh and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, Department of Microsystems Engineering (IMTEK), University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

Friction of a moving particle is a complex process of energy dissipation to the environment, which is important on most length scales, time scales and across disciplines. Several theories approach the molecular origin of friction, but a comprehensive understanding is still missing. Usually, the relation between dynamic friction and velocity is quantified by a coefficient, which depends on various parameters. Two main routes to determine the friction coefficient can be addressed by either from a directed particle motion or from its thermal motion. In both cases, Photonic Force Microscopy (PFM) has proven to be one of the most elegant techniques that can be utilized to better understand friction on mesoscopic length scales, specially at soft (-bio) interfaces. Towards this aim, we employ PFM with high-frequency axial tracking for directed and frequency dependent measurements of different bead-surface model systems, starting from simple poly-styrene (PS) bead-glass surface. From Brownian dynamics simulations, in combination with experiments, we obtain better insights on the friction coefficient and its dependency on different system parameters. From this, we developed a theoretical model describing the microscopic origin of friction through molecular on- and off-binding processes.

O 39.6 Wed 11:45 H6

Single Asperity Sliding Friction across the Superconducting Phase Transition — Wen Wang, •Dirk Dietzel, and Andrè Schirmeisen — Institute of Applied Physics, Justus Liebig University Giessen, Giessen, Germany

When analyzing sliding friction, it is usually an intriguing question to identify the different dissipation mechanisms contributing to friction. Usually, a number of different channels for dissipation are considered including phonon and electron systems, plastic deformation, and crack formation. Among these, especially the role of the electron system for energy dissipation often remains elusive. In this contribution, we now present experiments single asperity sliding friction monitored during AFM-measurements on a high-T_c BSCCO-superconductor. These measurements reveal a distinct temperature dependence of friction in a temperature range between 40 K and 300 K [1]. While the overall friction decreases with temperature as predicted by models about thermally activated friction, we find a distinct friction peak at about 95K. This peak can be explained by a superposition of different energy dissipation channels, where the influence of electronic contributions vanishes when cooling below the superconducting phase transition T_c. Our experiments thereby unambiguously link electronic friction effects to the number of normal state electrons in the superconducting phase below T_c. In addition, we analyze single asperity friction of BSCCO in the proximity of step-edges, where layer-defects reveal the potential influence of the topmost-layer on electronic friction contributions. [1] Wang, Dietzel, Schirmeisen, Science Advances, eaay0165 (2020)

O 39.7 Wed 12:00 H6

Fingerprint of a structural phase transition during superlubric sliding — •Ebru Cihan[1,2], Dirk Dietzel[1], and Andre Schirmeisen[1] — [1]Institute of Applied Physics, Justus-Liebig University Giessen, 35392 Giessen — [2]Institute for Materials Science, TU Dresden, 01062 Dresden

Although the fundamental concept of structural superlubricity (i.e. ultra-low friction observed between clean and atomically flat, incommensurate surfaces) is very straightforward, the effective energy barrier for lateral motion still depends on the exact structural dynamics at the sliding interface. In fact, it can be computationally predicted that the superlubricity of amorphous structures is less effective than that of crystalline structures, however this is not always easy to demonstrate experimentally. But we have now overcome this challenge by measuring the friction of antimony nanoparticles on highly oriented pyrolythic graphite in the high temperature regime, i.e. between 300 K and 750 K, where the interface can be restructured. At about 450 K, we trigger a phase transition in antimony nanoparticles, which also allows us to establish a direct link between friction and the interface structure. More specifically, our experiments reveal that the friction level decreases in the more crystalline state where the collective force cancellations are more effective. Due to the irreversible character of the phase transition, a reduced friction level can then also be observed after cooling back to room temperature. The reduction of friction can be associated with a decrease of the characteristic scaling factor of about 16%, as theoretically anticipated from the 'scaling law' for superlubricity.