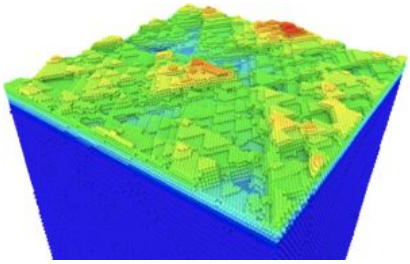
Workshop Report: Emergence of surface and interface structure from friction, fracture and deformation

Organisers: Lars Pastewka, Gianpietro Moras, James Kermode and Alessandro De Vita



The workshop on Emergence of surface and interface structure from friction, fracture and deformation, held at CECAM HQ in Lausanne from 24-27th July 2018, considered the topographic, morphological and chemical structure of surfaces and interfaces that arises from mechanical processes and how this structure affect the mechanical behaviour of materials but cannot typically be systematically controlled. As well as Psi-k, the workshop received support from CECAM, the DFG and EPSRC.

Few of the processes responsible for surface and interface structure formation are fully understood, often because they involve interactions across length and time scales. This topic was discussed from five perspectives:

1. **Structure of fracture surfaces.** This topic focused on the emergence of individual geometric features resulting from crack tip instabilities, such as oscillations of tip position in 2D or triangular protrusions found on a variety of materials in 3D, as well as the emergence of roughness on crack surfaces in glasses and hierarchical materials.
2. **Emergence of surface roughness during plastic deformation.** This was presented for metals and metallic glasses. Simulations showed the emergence of self-affine structures from homogeneous materials, and the creation of folds in polycrystalline samples. In experiments, surface and bulk deformation was visualized using metallic multilayers for contrast in microscopy or in-situ observation of surface cross-sections.
3. **Evolution of interface morphology during frictional loading.** This is intimately tied to plastic deformation and fracture. Observations of rock surfaces suggest a well-defined length-scale for the onset of brittle fracture. Simulations on 2D models show a similar transition and a potential explanation for these observations, pointing towards a unified wear model.
4. **Emergence of structure from elastic instabilities.** This was discussed in the context of folds and creases created during the deformation of soft solids.
5. **Chemical structure at surfaces and interfaces.** This was discussed in the context of fracture (hydrogen embrittlement) and friction (surface passivation during lubrication). Occurrence of tribochemical phenomena, and explicitly electronic-structure based simulations that reveal the relevant reaction mechanism were presented and amply discussed.

Outcomes of the workshop aligned with the five perspectives above include:

1. **Fracture.** During the workshop it became clear that a transition from understanding crack-path selection in two-dimensions to complex three-dimensional instabilities is underway. This poses a major challenge for experiments that typically look at post-mortem surface patterns after fracture has occurred in 3D, but often allow in situ observation in 2D. It is also a major challenge from a modelling point of view: most analytical models are derived for 2D and atomic-scale calculations are typically carried out in 2.5D. Multi-scale coupling relies to a certain extent on this 2.5D character because of the existence of small spatial regions to be modeled with accurate albeit expensive schemes. While these models can be even quantitatively predictive, there is a need for full 3D fracture simulations. It was demonstrated that both continuum scale phase-field models as well as large-scale atomistic models have started to bridge the gap from 2D to 3D models of fracture. There is a growing consensus that more work, requiring the incorporation of chemical and microstructural information into current models, is needed to identify the causes of geometric crack-path instabilities.
2. **Plasticity.** Experimental observation of pattern formation by plastic deformation on surfaces can be carried out in situ, but observation at interfaces (between grain boundaries or heterointerfaces) is presently limited to post-mortem analysis in oxidizing environments. The formation of folds is understood in terms of material heterogeneity (elastic and plastic moduli, Schmid factors) but novel results were presented that hinted at an influence of surface chemistry on these effects. Other phenomena, such as the formation of vortices during deformation, or the emergence of self-affine surface structure appear at present only to be understood in qualitative rather than quantitative terms.
3. **Friction.** Explaining frictional loading requires a combination of fracture and plastic deformation. While significant progress has been made in individual application areas (e.g., adhesive wear mechanisms), an overall systematic approach to scale-dependent strength is missing (see discussion of 'Grand Challenges' below).
4. **Elastic instabilities.** The formation of folds and creases ("rugae") during the deformation of soft solids can be well described by conventional continuum models. Plastic instabilities can of course never be completely decoupled from the effect of the elastic matrix, requiring more studies of the interplay of elasticity and plasticity.
5. **Chemical structure.** Coupling of chemical and mechanical models of fracture and friction shows great potential, with highlight applications making quantitative predictions linking modelling and experiment. However, as discussed in more detail below, the multiscale challenge of unifying accurate models of e.g. individual tribochemical processes with long-range driving forces in complex loading geometries remains as urgent as ever. However, direct coupling of models does little to address the time scale challenge.

As part of the workshop, we carried out a discussion session to assess the needs of the community, which as a result appear to include:

- The idea of 'virtual journals' organised by the community to collate relevant articles, with the goal of promoting the diffusion of high-quality work out of community journals. This is an activity which CECAM might be interested in promoting/facilitating, perhaps along with hosting the associated research data.

- Direct input from chemistry. When asked whom the participants would like to collaborate with but presently do not, the answer was overwhelmingly an expert in chemistry. This suggests that the community feels comfortable addressing mechanical aspects of structure formation but an understanding of chemomechanical effects is still in its infancy.

- Better integration with experimental activities. It was recognised that there is also a distinct difference between experimental and theoretical approaches. Theory always requires models, either generic ones that explain a certain process or material specific ones, experiments live in the real world and are often complicated, e.g. by ambient chemistry or mechanical noise. For model validation, there is a need for simpler (theory-led) experiments on ultra-pure samples of simplified composition/microstructure.

- Concrete recommendations for follow-up activities to nurture the burgeoning 'multiscale mechanics of interfaces' community include organising further workshops at CECAM, as well as proposing symposia at conferences such as MRS, MMM, DPG and EMRS. Setting up a COST action will also be explored.

- Interestingly, when asked about how the field could benefit from present prominent trends in data science, machine learning and artificial intelligence, participants said it is useful to develop methods and carry out high throughput screening of complex experimental results (e.g. spectra or fractographic images) but not as a general research approach in a community whose primary focus is elucidating mechanisms.

Commonly agreed limitations of existing funding instruments were identified:

1. Difficulting of initiating relatively small-scale research projects across national borders, e.g. modelling-experiment collaborations with 2-3 partners, where setting up a consortium under e.g. the LEIT Horizon 2020 actions would not be appropriate. More joint calls between national funding agencies, or a similar action facilitated by the EC, would help to address this concern.
2. Competition between long-term fundamental research and immediate practical needs - it can be difficult to demonstrate the impact of projects which focus primarily on method development, but which in the long term are expected to enable significant technical progress.
3. Concerns were raised that the current drive towards an open-access culture in particular at high-impact journals will make publishing in these journals impossible for a broad community of researchers because of the cost associated with it.

One of the discussion topics we asked participants to consider was the identification of 'Grand Challenge' problems that would bring the community together to tackle problems of pressing societal, economic and technological benefit, such as a mechanistic understanding of scale-dependent strength, requiring cross community engagement to address the multiscale competition between plasticity and cleavage. Progress is needed for societal challenges ranging from optimisation of nanoscale manufacture through to prediction of earthquakes.

Other challenges identified with important societal impact include an improved understanding of fracture of hydrogels, used for a wide range of applications including tissue engineering, drug delivery and biosensors; effects of environment on crack growth though stress corrosion cracking, relevant from biomedical implants to mining; optimising surface properties of high performance materials such as high entropy alloys and metallic glasses.

Moreover, all the topics discussed can also be exploited for manufacturing, where requirements on surface finish contribute a large proportion of the cost of a part. Being able to produce custom interfaces in materials by controlling chemistry and deformation during manufacturing would enable materials with tailored mechanical properties. Advanced manufacturing techniques may emerge from in-depth understanding of fundamental processes that shape surfaces in friction, fracture and deformation.

The participants were agreed that Psi-k and CECAM provide an ideal incubator/facilitator environment for creating the necessary interdisciplinary links, in a field with direct technological impact that only recently lends itself to detailed atomistic/molecular modelling, and can tap into expertise in materials (quantum) chemistry. On this basis, and looking ahead, the present set of organisers is contemplating planning another workshop, for 2020 (with detailed planning to be carried out in spring 2019).

Programme

Tuesday July 24th 2018 - Day 1
13:00 to 13:45 - Welcome and Introduction
13:45 to 14:15 - Lucia Nicola
14:30 to 15:00 - Adam Hinkle
15:15 to 15:45 - Coffee Break
15:45 to 16:15 - Dov Sherman
16:30 to 17:00 - Matthieu George

Wednesday July 25th 2018 - Day 2
09:00 to 09:30 - Ruth Schwaiger
09:45 to 10:15 - Herbert Urbassek
10:30 to 11:00 - Coffee Break
11:00 to 11:30 - Paolo Moretti
11:45 to 12:15 - Laurent Ponson
12:30 to 14:15 - Lunch

14:15 to 14:45 - Srinivasan Chandrasekar
15:00 to 15:30 - Stefano Zapperi
15:45 to 16:15 - Coffee Break
16:15 to 16:45 - Vikram Deshpande
17:00 to 20:00 - Poster Session with cold buffet sandwiches
Thursday July 26th 2018 - Day 3
09:00 to 09:30 - Kyung-Suk Kim
09:45 to 10:15 - Benny Davidovitch
10:30 to 11:00 - Coffee Break
11:00 to 11:30 - Jay Fineberg
11:45 to 12:15 - Alain Karma
12:30 to 14:15 - Lunch

14:15 to 14:45 - Emily Brodsky
15:00 to 15:30 - Ramin Aghababaei
15:45 to 16:15 - Coffee Break
16:15 to 17:00 - Discussion
19:30 to 22:00 - Social Dinner

Friday July 27th 2018 - Day 4
09:00 to 09:30 - Roberto Guerra
09:45 to 10:15 - Erik Bitzek
10:30 to 11:00 - Coffee Break
11:00 to 11:30 - Michael Moseler
11:45 to 12:15 - Closing Word

Presentation Abstracts

Modeling contact between metal bodies
Lucia Nicola
Delft University of Technology, The Netherlands

At moderate nominal contact pressure, only a small fraction of the surface asperities has to support all the load. This is why metal bodies deform plastically even when the nominal contact pressure is significantly smaller than the material hardness.
Although contact between elastic bodies has been studied extensively both analytically and numerically, little attention has so far been devoted to plasticity.

Here, we study plastic deformation starting from contacts with simple geometry, and move then to bodies with self-affine rough surfaces. The simulation technique used for simple geometries, namely flat asperities and sinusoidal surfaces, is discrete dislocation plasticity, in its small strain and finite strain formulation. In discrete dislocation plasticity, the plastic deformation of metal bodies is obtained by the collective glide of discrete dislocations, which nucleate from Frank-Read sources. Simulations show how plasticity induces surface roughening, and how asperities interact plastically.

Contact between self-affine rough surface is computationally more challanging and requires to use a computational method that allows for a detailed description of the surface roughness, spanning in lenght scale from 5nm to 100 micrometers. For this we developed a modeling technique that merges discrete dislocation plasticity with Green's function molecular dynamics. Green's function molecular dynamics is a boundary element method that gives a fast converging solution to elasticity problems exploiting the computational speed of fast Fourier transforms. It allows for a very fine discretization of the surface, and is here used to solve for the image fields of the dislocations.

Simulations are performed varying various parameters of the surface roughness, including the Hurst exponent and the root-mean-square height. Results show that the plastic response is size-dependent. An important implication of the size-dependence is that, when bodies deform plastically, it is not possible to scale observables such as contact pressure and contact area with crystal size or root-mean-square height, as typically done for elastic contact problems.

Emerging surface roughness during plastic deformation
Adam Hinkle
Sandia National Laboratories, USA

Most natural and man-made surfaces appear to be rough on many scales. However, there is presently no unifying theory of the origin of roughness or the self-affine nature of the surface topography. This talk explores the role of mechanical deformation upon the formation of surface roughness. In particular, the plasticity observed in mechanically driven amorphous and crystalline solids has been characterized by avalanches of irreversible rearrangements exhibiting a self-affine, power-law behavior. Using molecular dynamics we simulate the bi-axial compression of a metallic glass and a single crystal of gold. We extract the free surfaces during the deformation and characterize the roughness and self-affine

character. Analysis of the power spectral density reveals Hurst exponents above 0.5 for both the amorphous and crystalline surfaces, and a similar self-affine scale invariance is found within the displacement correlations of the bulk during plastic deformation.

Dynamic fracture surface instabilities in brittle crystals
Dov Sherman, Liron Ben-Bashat Bergman
Tel-Aviv University, Israel

Fracture surface instabilities in form of micron scale ridges were evident on the (111) low energy cleavage plane of B doped silicon crystal under 3-Point-Bending and under tension, at relatively low crack speed [1,2]. The ridges density increases as B density increased (3,4). The origin of these ridges was found to be an atomistic scale jogs occurring when the dynamic crack collided with a single B atom [3,4]. Jogs were pile-up to initiate the micron scale ridge. Recently, we generalized the phenomenon by cleaving cubic silicon (doped with B, O, and P) and germanium (doped with Ga) crystals for cracks propagated on the (111) [11] low energy cleavage system [5].

A continuum based theoretical model was developed [5], based on energy minimization law; at certain crack speed and chemical local strain energy induced by a dopant, the crack will deflect to generate an atomistic height wedge like jog (like in dislocations) while diminishing the local chemical strain energy. The model predicts the crack speed at jog generation. The major outcome of the model is that even the densest jogs have only limited influence on crack speed. The surface instabilities on the of (110) cleavage plane of silicon crystal do not develop to form ridges. New investigation of crack propagation on 3 cleavage systems of LiNbO3 crystal show no surface instabilities in form of ridges, presumably due to the complex atomistic arrangement, which regulates and stabilizes the crack path. We postulate that ideal brittle crystals with no dopant (no such a crystal was found) would be stable and smooth at low (excluding 'Wallner lines") and at high speed.

[1] D. Sherman, M. Markovitz, and O. Barkai, JMPS 56, 376-387 (2008).
[2] J.R. Kermode, T. Albaret, D. Sherman, N. Bernstein, P. Gumbsch, M.C. Payne, G. Cs´anyi, and A. De Vita, Nature 455, 1224-1227 (2008).
[3] J.R. Kermode, L. Ben-Bashat Bergman, F. Atrash, J. J. Cilliers, D. Sherman, and A. De Vita. Nature Communication 4, 2441 (2013).
[4] L. Ben-Bashat Bergman and D. Sherman, Scripta Materialia 75, 14-17 (2014).
[5] L. Ben-Bashat Bergman and D. Sherman, submitted (2018).

Roughness of oxide glass sub-critical fracture surfaces. How to measure and how to interpret?
Matthieu George, Gael Pallares, Frédéric Lechenault, Matteo Ciccotti
University of Montpelier, France

An original setup combining a very stable loading stage, an atomic force microscopy and an environmental chamber, allows to obtain very stable sub-critical fracture propagation in oxide glasses under controlled environment, and subsequently to finely characterize the nanometric roughness properties of the crack surfaces.

In this presentation, I will focus, on one hand, on the special experimental care that has to be devoted to measure the metrological properties of such nanometric rough surface by

Atomic Force Microscopy (AFM) and, on the other hand, on the interest of analyses in terms of physical indicators related to the self-affine nature of the fracture surfaces.

Due to the comparable nanometric amplitude of the surface roughness, the AFM tip size and the instrumental noise, it seems interesting to discuss about potential experimental artefacts highlighted by Lechenault et al [1].
The roughness amplitude of several oxide glasses was shown to decrease as a function of the stress intensity factor, to be quite insensitive to the relative humidity and to increase with the content of network modifiers [2]. These results will be discussed in terms on several modellings concerning the coupling between crack propagation, material heterogeneity, crack tip plastic deformation and water diffusion at the crack tip taking into account the self-affine nature of the fracture surfaces.

[1] F. Lechenault, G. Pallares, M. George, C. Rountree, E. Bouchaud, M. Ciccotti. Effects of Finite Probe Size on Self-Affine Roughness Measurements. PRL 104, 025502 (2010)

[2] G. Pallares, F. Lechenault, M. George,E. Bouchaud, C. Ottina, C. L. Rountree, M. Ciccotti. Roughness of oxide glass subcritical fracture surfaces. J. Am Ceram Soc. 2018;101:1279–1288 (2018).

Microstructural changes of metallic nanolayered composites under cyclic sliding
Ruth Schwaiger
Karlsruhe Institute of Technology, Germany

Nanoscale metallic multilayers represent a new class of engineering materials with superior physical and mechanical properties. Previous investigations have illustrated that deformation and strength of multilayers depend on the layer thickness and the type of interface between the layers, which directly controls the barrier strength of the interface and the stability of the multilayer structure under mechanical loads. In particular, this structural stability is critical to the performance of multilayer materials under sliding contact since deformation-induced microstructural changes may affect the subsequent wear response of the materials.

In this study, nanoscale metallic multilayers with different types of interfaces were investigated. Sliding experiments at different normal loads with up to 1000 cycles were conducted using a nanoindenter equipped with a spherical tip. The microstructures underneath the sliding tracks were investigated by scanning and transmission electron microscopy. The thinner layers exhibit improved wear behavior. Pronounced microstructural changes were observed such as deformation-induced grain growth, layer thinning and microstructural vortices. The effect of the type of interface and layer thickness on the deformation and wear behavior will be presented.

Plasticity under nanomachining: atomistic simulations
Herbert Urbassek
University of Kaiserslautern, Germany

Machining of surfaces has been studied by atomistic methods for the cases of nanoindentation, scratching, and cutting. When machining surfaces of ductile materials plastic zones are created around the machined regions. Starting with the comparably well

understood process of nanoindentation, we characterize the plastic zones created by nanoscratching. We find that the plastic zone sizes after scratch are comparable to those after indent. Due to dislocation reactions, the dislocation networks simplify, reducing the total length of dislocations. As a consequence, the average dislocation density in the plastic zone stays roughly constant. Individually, we find exceptions from this simple picture. Fcc metals show strong plastic activity, which even increases during scratch. The hcp metals on the other side show the least plastic activity. Here the plasticity may be strongly reduced during scratch and particularly during tip withdrawal.

Super-rough crack morphology in materials with hierarchical microstructures
Paolo Moretti, Bastien Dietemann, Nosaibeh Esfandiary, Michael Zaiser
University of Erlangen-Nurenberg, Germany
University of Erlangen-Nuremberg

Hierarchically patterned microstructures are often encountered in materials of biological relevance, including collagen, nacre and wood. The hierarchical organization is believed to entail crack confinement and enhanced fracture toughness. We propose two- and three-dimensional numerical models of fibrous biological materials under load, accounting for the hierarchical nature of their microstructures and their intrinsic heterogeneity. We show that hierarchical spatial patterns are responsible for the emergence of complex super-rough crack surfaces, characterized by large deflections, which appear in agreement with the crack shapes encountered in bone fracture. We find that failure in these systems is not accompanied by the growth of a critical crack surface, as crack growth is constantly hindered by the materials microstructure. We highlight that this unusual fracture mode is accompanied by a generic precursory activity, in the form of stress and strain avalanches with heavy-tailed distributions of sizes, not just at the peak load, but throughout the entire loading curve.

Triangular fracture patterns in polymeric materials as the signature of shear induced crack-front instability
Laurent Ponson, Aditya Vasudevan, Alain Karman, Jean-Baptiste Leblond
Université Pierre et Marie Curie, France

Fractography, the study of fracture surfaces, is a broadly used engineering technique that aims at tracing back the history of a failure and determining its root causes. For 30 years, the study of fracture patterns has taken a new turn: could we learn from the morphology of fracture surfaces the fundamental laws that govern the behavior of cracks?

During this presentation, I will present some remarkable advances in the understanding of triangular fracture patterns observed on fracture surface of polymeric materials. I will show how these patterns emerge from the fragmentation of the crack-front in small facets resulting from the presence of shear.

This study will lead us to revisit the roughening instabilities that may take place in presence of mode II and mode III during dominantly mode I fracture, and explain why they can take place even at very low levels of shear. Our findings suggest that shear induced facets are ubiquitous in tensile fracture and that similar patterns observed in a wide range of materials may be related to the same instability.

Stability of surface plastic flow in shear deformation of metals

Srinivasan Chandrasekar, Koushik Viswanathan [1], Anirudh Udupa [1], Tatsuya Sugihara [2], James Mann [3]
Purdue University, USA
[1] Center for Materials Processing and Tribology, Purdue University, Indiana, USA; [2] Osaka University, Osaka, Japan; [3] University of West Florida, Pensacola, Florida, USA

We examine stability of surface plastic flow in shear deformation of soft and highly strain hardening metals, using high-speed in situ imaging and ex situ characterization techniques. The shear is imposed by a sliding wedge indenter – an asperity - in configurations reminiscent of cutting and sliding. In addition to the well-known homogeneous/smooth plastic flow, three unsteady flow modes are identified on the mesoscale, each with distinct characteristics. We show that these surface flow modes are determined primarily by stability criteria, and are directly correlated with morphology of wear particles or chips. Attributes of a recently uncovered mode of unsteady flow – sinuous flow – characterized by large-amplitude material folding are discussed in detail. Transitions between the four flow modes are demonstrated, and are effected by changing the deformation geometry or the initial material state. Lastly, a coupling between mechanochemical effects at surfaces and unsteady flow is demonstrated and analyzed within the framework of flow stability. We present a phase diagram that describes the effects of deformation geometry and material state on the flow modes. The diagram also naturally accounts for the flow transitions observed in the experiments. Implications for manufacturing processes, sliding wear and surface engineering will be highlighted.

Atomic-Scale Front Propagation at the Onset of Frictional Sliding

Stefano Zapperi, Silvia Bonfanti, Alessandro Taloni, Carlotta Negri, Alessandro L. Sellerio, Nicola Manini
University of Milan, Italy

Macroscopic frictional sliding emerges from atomic-scale interactions and processes at the contact interface, but bridging the gap between micro and macro scales still remains an unsolved challenge. Direct imaging of the contact surface and simultaneous measurement of stress fields during macroscopic frictional slip revealed the formation of crack precursors, questioning the traditional picture of frictional contacts described in terms of a single degree of freedom. Here we study the onset of frictional slip on the atomic scale by simulating the motion of an aluminum block pushed by a slider on a copper substrate. We show the formation of dynamic slip front propagation and precursory activity that resemble macroscopic observations. The analysis of stress patterns during slip, however, reveals subtle effects due to the lattice structures that hinder a direct application of linear elastic fracture mechanics. Our results illustrate that dynamic front propagation arises already on the atomic scales and shed light on the connections between atomic-scale and macroscopic friction.

Hydrogen induced fast fracture

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One of the recurring anomalies in the hydrogen induced fracture of high strength steels is the apparent disconnect between the toughness and the tensile strength of un-notched bars. For example, the toughness of a high strength steel is typically reduced from 100 MPa$\sqrt{m}$ to about 20 MPa$\sqrt{m}$ in the presence of hydrogen while concurrently the strength reduces from 2 GPa to about 400 MPa. Traditional fracture mechanics then suggests that quasi-brittle fracture of the tensile bar occurred to growth of a crack from a pre-existing flaw of size ≈1600 μm. There is no evidence of the presence of such large pre-existing flaws in high quality steels. This raises the question as to what is the hydrogen-mediated fracture process that reduces the strength of such steels?

Here we present a model for hydrogen induced fast fracture that attempts explains this disconnect. Using a combination of atomistic calculations as well as continuum plasticity and fracture analyses, we illustrate that cracks can grow rapidly from small flaws such as voids within the steels (these voids can be pre-existing or nucleate and grow around inclusions such as carbide particles). The rapid growth of these cracks is fed by hydrogen within the void with the fast crack growth suppressing plasticity around the crack tip. However, this hydrogen-fed fast crack growth can typically grow cracks by no more than 10 μm after which hydrogen from within the void is depleted. Here we show via coupled continuum plasticity and fracture calculations that this fast crack growth can persist, now in the absence of hydrogen, even at relatively low levels of remote applied load. It is this continued fast crack growth, and the consequent suppression of plasticity, that results in the brittle fracture of the tensile bars. Thus, we argue that fracture within the tensile bar occurs via a fundamentally different process to the slow crack growth in toughness measurements – it is this difference in modes that gives rise to the anomaly mentioned above. The model is used to explain a host of well-established experimental observations including: (i) in insensitivity of the strength of the concentration of trapped hydrogen; (ii) decrease in the tensile ductility with increasing hydrogen concentration and (iii) why hydrogen embrittlement is seldom observed in low strength steels.

Hidden, forbidden and inherited spectrum of roughness caused by multilayer deformation instabilities near a free surface

Kyung-Suk Kim
Brown University, USA

Solid-surface roughness can be produced by many different mechanisms such as crack-front growth instabilities, stress-assisted diffusion-driven evolution instabilities, stress-assisted deposition or erosion instabilities, and chattering instabilities of friction, etc. In addition to these mechanisms, multi-layer structure with varying modulus is unstable under lateral compression, and near-surface layer deformation instabilities can generate hierarchical spectrum of roughness on the surface. Here, we introduce mathematical modeling of multilayer deformation instabilities near a free surface, that cause hidden, forbidden and inherited spectrum of roughness on the surface. The mathematical modeling is experimentally verified by hierarchical wrinkles with wavelengths that span several orders of magnitude on a polydimethylsiloxane (PDMS) surface treated with UV/Ozone. In the experimental study, we show that originally homogeneous PDMS develops a structure whose elastic modulus varies as a function of depth from the free surface upon treatment with UV/Ozone. This multi-layer structure with varying modulus is responsible for the formation of hierarchical wrinkle structures. Revealing the intrinsic link between the variation of the material properties and the multi-scale wrinkling instability can help

scientists and engineers understand a formation mechanism of broad-scale surface roughness spectrum on a solid surface.

Geometrically incompatible confinement of thin elastic bodies
Benny Davidovitch
University of Massachusetts-Amherst, USA

Confining thin objects, such as rods, sheets and shells into a volume smaller than their lateral size typically generates in them stress. Relaxation of this stress often gives rise to the formation of complex patterns – wrinkles, crumples, folds, and so on. This general description spans a broad range of natural phenomena, such as tissue-shaping instabilities in animal epithelia, plant leaves, and perhaps even the formation of brain sulcus. In this talk I will describe a variational approach to the confinement of thin elastic bodies that encompasses the mechanical and geometrical routes through which confinement gives rise to elastic instabilities and pattern formation phenomena.

The topology and mechanics of the formation of fracture surface patterns
Jay Fineberg, Itamar Kolvin, Mokhtar Adda-Bedia
Hebrew University, Jerusalem, Israel

How and why are patterns formed on broken surfaces? Faceted fracture surfaces are commonly formed by slow tensile cracks in amorphous materials; hence their formation cannot reflect microscopic order. While fracture mechanics predict that slow crack fronts should be straight and form mirror-like surfaces, facet-forming fronts propagate simultaneously within different planes separated by steps. Why are steps stable, what determines their path and how do they couple to crack front dynamics? By integrating real-time imaging of propagating crack fronts with surface measurements, we demonstrate that steps are topological defects; crack front separation into disconnected overlapping segments provides the condition for step stability. Crack dynamics are enslaved to steps; steps drift at a constant angle to the local front propagation direction while their increased dissipation couples to long-ranged elasticity to determine front shapes. We see how 3D topology couples to 2D fracture dynamics to provide a fundamental picture of how patterned surfaces are generated. We also show that crack front curvature may feed back to deflect step paths via nonlinear focusing of crack fronts, causing steps to converge to form a micro-branch. Thus, our results supply the basis for a unified picture of pattern formation on fracture surfaces.

Fracture Patterns from Symmetry-Breaking Instabilities in Homogeneous and Composite Materials
Alain Karma
Northeastern University, Boston, USA, USA

This talk will discuss recent progress to understand complex fracture patterns arising in homogeneous and composite materials from various symmetry-breaking instabilities of propagating cracks. Three main topics will be discussed that include the oscillatory instability of ultra-high-speed cracks, crack-front segmentation and coarsening under the superposition of tension and antiplane shear (mixed mode I+III loading), and crack kinking in anisotropic biomimetic composites. Results will be presented that highlight how progress on each topic has been achieved by quantitative comparisons between experiments and theory, including

numerical simulations of crack propagation using the diffuse-interface phase-field method and theoretical analyses in the classical framework of linear elastic fracture mechanics.

The Minimum Scale of Grooving on Faults
Emily Brodsky
University of California-Santa Cruz, USA

At the field scale, nearly all fault surfaces contain grooves generated as one side of the fault slips past the other. Grooves are so common that they are one of the key indicators of principal slip surfaces. We have shown that at sufficiently small scales, grooves do not exist on fault surfaces. A transition to isotropic roughness occurs at 4–500 μm. Although the scale of the transition can vary even between locales on a single fault, the aspect ratio of the roughness at the transition is well defined for a given fault. We interpret the transition between grooved and ungrooved scales as a transition in deformation mode of asperities on the slip surface. Grooves can form when a hard indenter slides past a softer surface. At small scales, the asperities appear to yield plastically and therefore do not generate grooves as hard indenters. The plastic yielding can be a consequence of the high shear strains required to deform the surfaces at small scales where the aspect ratio (roughness) is high. The transition to plastic yielding is predicted to occur at a specific aspect ratio for each fault, as observed. The new observation both shows a limit to one of the most commonly observed features of faults and suggests a change in the mode of failure of faults as a function of scale.

Surface roughness evolution during wear processes
Ramin Aghababaei, Jean-Francois Molinari, Enrico Milanese, Tobias Brink
Aarhus University, Denmark
EPFL, Switzerland
Material surfaces are rough at all magnifications, ranging from atomistic to macroscopic scales. Roughness evolution is of critical importance in many applications, including tribology and machining processes. During sliding contact, surface asperities interact and form tiny junctions. Failure mechanisms of these asperity junctions dictate frictional and wear responses of surfaces and the surface roughness evolution. How does the surface profile govern junction failure mechanisms and vice versa? Here we present coarse-grained atomistic simulations and complementary model experiments of asperity junction failure during sliding contact.

Results show that bulk and interfacial properties of sliding surfaces and topology of surface roughness determine a critical length-scale that dictates failure mechanisms of adhesive asperity junctions. Brittle (sudden) versus ductile (gradual) failure mechanisms, resultant force profiles, and changes in surface roughness are discussed. Tracking surface roughness evolution in long-timescale simulations shows that the emergence of self-affine surfaces is governed by the interplay between the ductile and brittle failure mechanisms, and is independent of the initial state. Accounting for both mechanisms and the third body is, therefore, necessary to investigate the physics of roughness evolution, from the nanoscale to the geological scale.

Our simulations also show that the asperity junction size dictates wear particle size, revealing the origins of the long-standing hypothesized correlation between the wear volume and the real contact area (i.e. Archard's wear law). However, a recent investigation of sliding contact beyond single-asperity level shows that the interaction between neighboring asperity junction triggers the deep propagation of subsurface cracks and the

eventual detachment of large wear particles, with a size corresponding to an effective apparent and not the real contact area of neighboring asperity junctions. This observation might explain the breakdown of the linear relation between the wear volume and the normal load in the severe wear regime.

Damage accumulation in silica glass nanofibers
Roberto Guerra
University of Milan, Italy

The origin of the brittle-to-ductile transition, experimentally observed in amorphous silica nanofibers as the sample size is reduced, is still debated. Here we investigate the issue by extensive molecular dynamics simulations at low and room temperatures for a broad range of sample sizes, with open and periodic boundary conditions. Our results show that small sample-size enhanced ductility is primarily due to diffuse damage accumulation, that for larger samples leads to brittle catastrophic failure. Surface effects such as boundary fluidization contribute to ductility at room temperature by promoting necking, but are not the main driver of the transition. Our results suggest that the experimentally observed size-induced ductility of silica nanofibers is a manifestation of finite-size criticality, as expected in general for quasi-brittle disordered
networks.

Influence of Interface Curvature on Deformation and Fracture
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Interfaces play a decisive role in the deformation and failure of any polycrystalline metal, precipitate-strengthened alloy or surface-dominated nanoobject. The underlying mechanisms like dislocation – grain boundary (GB) interactions (including dislocation absorption and pinning), crack initiation and grain boundary fracture, precipitate cutting, or nucleation of dislocations at surfaces all take place at the atomic scale. Consequently, atomistic simulations have played a key role in studying grain- and interphase boundaries (IPBs). However, in many of these studies, the interfaces are idealized as perfectly planar, and often infinite, interfaces.
In this talk, we compare atomistic simulations of dislocation – GB interactions, nanocrystal deformation, misfit dislocation network formation in fcc metals with planar and curved interfaces. Straight, infinite dislocations interacting with curved grain boundaries showed dislocation pinning but also a decreased critical resolved shear stress compared with a planar GB of identical misorientation. Al nanocrystals with grain morphologies obtained from grain growth simulations (allowing for GB curvature) showed deformation twinning, which is not observed in Voronoi-tessellated samples (that enforce planar GBs), although they have similar distributions of grain sizes and number of faces per grain. We also studied systematically the misfit dislocation network that develops in model Ni-base superalloys when joining the L12 Ni3Al γ'-phase to the fcc Ni γ-phase for different degrees of IPB curvature. Here, the misfit dislocation core structure as well as misfit dislocation network topology critically depend on the curvature. Simulations using experimentally-obtained precipitate morphologies demonstrated that these changes result in pronounced differences when the interaction of matrix dislocations with the precipitate is studied. We furthermore report on investigations of straight and curved cracks in bcc single-crystals and along GBs and conclude with a recent study of fracture along curved GBs.

Formation of superlubricious layers by mechano-chemical decomposition of lubricants with multiple reactive centers

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Superlubricity has been observed for tetrahedral amorphous carbon (ta-C) coatings lubricated with unsaturated organic friction modifiers or glycerol but the underlying mechanisms remain elusive. Here, combined experiments and simulations unveil the tribochemical mechanism leading to superlubricity of ta-C/ta-C tribopairs. Pin-on-disc sliding experiments show that super- and ultralow friction with negligible wear can be achieved by lubrication with unsaturated fatty acids or glycerol, but not with saturated fatty acids and hydrocarbons. Atomistic simulations reveal that, due to the simultaneous presence of a carboxylic group and a C=C double bond, unsaturated fatty acids can concurrently chemisorb on both ta-C surfaces and bridge the tribogap. The resulting, sliding-induced mechanical strain triggers a cascade of molecular fragmentation reactions that release passivating hydroxyl, keto, hydrogen and olefinic groups to the ta-C surfaces. Simulations for glycerol show that all three hydroxyl groups can be considered reactive centers that bind to both surfaces, induce cold welding followed by the formation of aromatic passivation layers with superlow friction. These findings provide design principles for novel organic friction modifiers that promote the formation of superlubricious and wear-protecting, oxygen-containing amorphous carbon layers.

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