Research Statement

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My general scientific interest is in applications of statistical approaches to multiscale problems in material science and mechanics. In both experiments and theory, the aim is always towards identifying new classification principles of large ensembles of data, in order to build insightful minimal models and possibly, capture universal, across scales, aspects of complex material behaviors. The major target is to provide uncertainty quantification for large data sets and novel data science approaches.

Papanikolaou’s group uses statistical theory and several scientific computing techniques to study pattern formation phenomena, including: Monte Carlo for lattice models (dimers/spins), Discrete element Modeling (Jamming/Crowd dynamics, Discrete Dislocation Dynamics), Cellular Automata Modeling (crystal/amorphous plasticity) and Finite Element Analysis (basic crystal elasticity/plasticity algorithms).

The current 5-year plan involves two broad topics that are described below:

A. Uncertainty quantification, data science and collective phenomena in materials during mechanical deformation, with particular focus on near-boundary crystal plasticity and nanoindentation phenomena.

B. Statistical mechanics and pattern formation in highly frustrated systems with potential applications on jamming of sandpiles under stress (and other similar geophysical contexts), crowds during room evacuation, neuronal activity.

The group’s research program is funded by multiple active grants, which should probably be renewable for at least the next 10-15 years:

1. DOE-BES: $585,000 lead-PI (with Co-PI K. Hemker) grant from the Department of Energy – Basic Energy Sciences, Mechanical Behavior and Radiation Effects (2015-2018)
2. NIST: $160,000 personal grant from the National Institute of Standards and Technology – (2015-2018)
4. VIDI-NWO: €800,000 early-career excellence grant (VIDI) from the Netherlands Research Council (NWO) (2014-2019) – currently assigned to University of Groningen, Zernike Institute for Advanced Materials, with my required scientific leadership and co-supervision with E. Van der Giessen.

Moreover, several pending proposals may be funded in the ongoing academic year:

• ARO Lead-PI Grant (with B. Aguirre, J. Mitrani, J. Epstein, H. Egeth): Minimal agent-based models and passive warning systems in evacuating crowds. ($400,000, 2016-19)
• JHU-KSAS Faculty Innovation co-PI Grant (with E. Niebur, S. Sun, A. Kirkwood, H. Lee): Understanding the physiological basis of acute concussion. ($385,000, 2016-19)
• DOE-BES, Joint-PI Grant (with B. Marsh, M. Hilpert): Permeability and dynamics in fractured granular materials: Experiments and theory as function of polydispersity and granular volume fraction. ($425,000, 2016-19)
• NSF Personal Grant: Universal aspects, analogies and optimization of the mechanical response of amorphous complex systems: From micro-crystals and metallic foams to biological networks and granular systems. ($375,000, 2016-19)

The basic summary of the principal research directions are described below:

A. Collective phenomena, uncertainty quantification and data science in materials during mechanical deformation: The mechanics of deformed crystals may become unconventional and stochastic either at the nanoscale or when the deformation takes place near boundaries – possibly microscopic. Modeling approaches in these regimes depend not only on their derivation’s rigor but also on insights from detailed experimental efforts. Papanikolaou’s group aims at developing minimal, reduced-order models towards a two-fold goal: First, to guide intelligent classification /organization schemes for large data sets on polycrystalline or composite materials, based on insightful physical arguments, properly defined order parameters and statistical correlations; Second, to develop rigorous coarse-graining approaches for detailed multi-parameter computational models. The group’s current focus is on the elastoplastic deformation of near-boundary regions: 1. Free boundaries of nanopillars (DOE-BES): There has been significant interest in the uniaxial deformation of nano-scale pillars that are typically constructed using the FIB-technique. In a sequence of works, Papanikolaou’s group has been building a complete theory of nanoscale plasticity that includes both unconventional strengthening and statistical collective mechanisms of plastic deformations. 2. Grain boundaries in thin films (DOE-BES/NIST): One of the major challenges in modeling continuum crystal plasticity is the role of grain-boundaries during plastic deformation. Papanikolaou’s group has designed a multi-axial stress setup of thin-film 4-point bending, where nanoindentation is analyzed as a function of the local granular structure in simple metals(Cu and Al). This relatively modest experiment, apart from answering concrete fundamental questions on plasticity dynamics, will serve as a playground for developing models and a library of statistical, dynamical correlations in polycrystalline plasticity. 3. Plastic zone of short fatigue-driven cracks(AFOSR): Papanikolaou’s group investigates the statistical character of the slow growth and propagation of cracks, developing protocols and minimal models. While no specific material is preferred, current efforts are concentrated in thin-films of ceramics and Ni-superalloys.

B. Statistical mechanics and pattern formation in highly frustrated dynamical systems: Frustration naturally emerges when driven particles/agents are spatially constrained, leading to “kinetic arrest” or jamming. Jamming may take place, under specific circumstances, in a large collection of systems and it represents the most direct example of the formation of mechanically stable but disordered microstructures. Papanikolaou’s group investigates the possibility that there are universal connections, in physical observables, among seemingly very different systems that undergo jamming: 1. Vibrations of jammed granular piles (VIDI-NWO): Papanikolaou’s group has developed the “Geometric Asperity” model of jamming of polydisperse disks, a useful approach to understanding the role of friction in statics and dynamics of disordered assemblies. Papanikolaou’s group investigates the vibrations and mechanical deformation of such assemblies in detail, 2. Crowd evacuation dynamics near
doors (ARO-pending): The motion of a crowd during room evacuation is analogous to jammed hopper flows. Papanikolaou’s group develops models and validates them (in collaboration with J. Mitrani’s Civil Eng. JHU group) for understanding pattern formations and possible optimizations in crowd evacuation time without structural motifs, 3. Cytoskeleton networks under shear (VIDI-NWO): Inside living cells, the role of a highly-disordered network of actin filaments appears to be crucial for understanding living processes. Papanikolaou’s group investigates the deformation of a few actin filaments in the presence of realistic on-off dynamics of inter-actin cross-linkers.

DOE Lead-PI Grant #DE-SC00014109 (2015-2018)
NANOindentation of micrograins in polycrystals under multiaxial stress: Control of abrupt & stochastic plastic events

Deforming objects in the world of the small has proven a much more complex task than just bending a common-sized object like a spoon. Over the last decade, it has become clear that the application of stress on micron-sized objects, such as micropillars, leads to abrupt and stochastic plastic strain jumps that do not satisfy Weibull statistics (as expected for uncorrelated defect yielding) but instead seem to follow highly wide, power-law distributions, pointing towards cooperative dislocation plasticity. Are power-law distributed plastic events the rule or the exception in crystals? If the rule, can we design protocols to control and suppress them in order to achieve deterministic and smooth microforming processes?

We combine experiments and theory to unravel the mysteries of abrupt microplastic deformation in a natural dislocation environment: micron-sized grains (“micrograins”) of polycrystals. We use a novel experimental design that utilizes nanoindentation and 4-point bending techniques on the substrate of polycrystalline thin films of two typical FCC metals (Al and Cu), and make concrete theoretical conjectures, based on intuition built from previous theoretical and experimental efforts in micropillar compression and nanoindentation.

Based on a wide set of observations over the last decade, we put forward two distinct hypotheses that we propose to investigate in both theory and experiments:

Our first conjecture is that crystal plasticity in the central region of micron-sized grains has micropillar-like stochastic features: power-law plastic strain jumps at stresses above the macroscale yield strength, displaying strong size and rate effects. We aim to demonstrate this similarity in spherical nanoindentation experiments in the central-region of multi-orientation grains of Al and Cu thin films. Al and Cu are selected for their disparity in stacking fault energy and consequently, their different propensity for cross-slip relaxation; however, our protocol may be applied to any crystalline material of technological interest. We will test our hypothesis by performing two-dimensional extended discrete dislocation plasticity (2D-DDP) simulations, inspired by comparable successful studies of micropillar plasticity, and extended to model nanoindentation with two slip systems and on a surface of a bicrystal with microhard grain-boundaries (GB), ie.not allowing dislocation absorption (116). Our model will include effective three dimensional dislocation mechanisms such as dislocation multiplication and double-cross-slip assisted glide.

Second, we hypothesize that the application of uniform in-plane stress on our thin films below the yield point can smoothen the micrograin plastic response during nanoindentation. On a tech-
nological level, we propose that indentation-induced localization (sink-in) may be diminished by the application of concurrent in-plane stress that activates slow, viscoplastic relaxations near GBs. We aim to demonstrate our hypothesis through a 4-point bending apparatus that introduces a homogeneous in-plane stress state before indentation. We will perform simulations of a coarse-grained mesoscale theory of plasticity in a system with microhard GBs, benchmarked through 2.5D-DDP simulations, which will capture the effects of slow viscoplastic relaxations.

**NIST Personal Grant # 70NANB15H230 (2015-2018)**

**Identifying dislocation plasticity laws from microscopic principles using experimental imaging: Examples near boundaries**

The main problem of elastoplastic features of material boundaries is that there is no apparent “universal” form of their response to simple shear: Depending on the case, grain boundaries may slide, migrate, behave as obstacles to dislocation motion, lead to dislocation nucleation or remain transparent to dislocations; (1) substrates can increase the size of the dislocation core in impressive fashion (2) and may or may not provide obstacles for dislocation motion; (3) inclusions in composite materials can have a wide range of elasto-viscoplastic responses to deformation. (4) There is currently no well accepted way to make predictions (for constitutive elastoplastic laws) that may be functional across boundary types that dislocations may encounter during their motion.

We are focused on identifying experimentally-inspired approaches to build continuum constitutive laws that describe the behavior of elastoplastic materials near boundaries: We consider example test-cases that involve the deformation behavior of: a. bicrystals with grain-boundaries, (1) b. thin crystalline films on substrates with various hardening effects, (3) c. composite materials in various geometries (cylindrical, rectangular inclusions).

The fundamental theoretical problems arising near boundaries can be summarized in that: i) The full plastic distortion information cannot be experimentally identified, typically only misorientation content can be typically quantified with available techniques, ii) Continuum plasticity theories near boundaries (strain-gradient theories SGT) are applicable only on a case-by-case basis given their complexity and the multiplicity of their assumptions.

In all examples to be studied, we will consider that the misorientation content is provided by experimental micrographs (for example, Transmission Electron Microscopy (TEM)) at several stages of the prescribed plastic deformation. Then, our playground of discrete dislocation dynamics (DDD) will be implemented to “interpolate” across strain and explain the micrograph strain evolution. We will investigate the extent of applicability of Principal Component Analysis (PCA) techniques in identifying features of elastoplastic deformation using a diverse set of utilized observables. Further, in order to improve the predictive ability of the DDD simulations, we will investigate the possibility of parameter optimization: E.g. 1. Distribution of Frank-Read dislocation sources on boundary, 2. Distribution of dislocation obstacles on boundary, 3. Distribution of statistically stored dislocation dipoles across the sample in the start of the simulation, as well as other parameters of the simulation. Our experimentally benchmarked DDD simulation approach can be also compared to several continuum SGTs for the behavior near boundaries. We aim to
implement DDD and several available SGTs in the context of the OOF2 package (Finite Element Analysis of Microstructures) developed by NIST. Ultimately, due to Python flexibility, our work provides a tool to compare continuum and discrete plasticity models in real-time dynamics with spatial resolution. All our results and methods will become ultimately generalizable to three dimensional models.

AFOSR Personal Grant #S-992-009-001 (2015-2019)

Plastic Deformation at the mesoscale and its importance during short-crack growth

We explore aspects of plastic deformation of structural metals that are limiting their application in advanced aerospace systems. We focus on the strengthening effects produced by complex chemistries and precipitates in new and existing high temperature structural materials, deformation mechanisms in bcc and fcc High-Entropy alloys, dislocation-precipitate reactions during creep in Ni-based superalloys and short crack growth.

We plan to explore the nature of plastic deformation at the atomic scale to ascertain the intrinsic length scales that emerge at or below 50 micron. Such scale dependent flow shall be modeled (using primarily discrete dislocation dynamics simulations) and will be compared to measurements of micro compression or tension methods. Further, we aim to explore the nature of short crack growth using novel micro, milli or macro scale testing methods in structural metals. The statistics of experimental data on crack growth and energy release as a function of stress, strain, strain rate, time and fatigue cycle rate will be assessed and analyzed.

We will use discrete dislocation dynamics modeling coupled to Finite Element Analysis to track the evolution of short cracks due to plastic deformation. We will constrain ourselves to a two-dimensional system and straight edge dislocations, the simplest possible system for this purpose, which can explore more efficiently longer timescales. Through such modeling we aim to explore different loading conditions and their possible effects. The approach/codes we will use are based mainly on well known methods. Our simulations will be compared to carefully designed experiments that emulate the simulation approach. Our target is to align, with time, our experimental and theoretical efforts towards clear and unambiguous comparisons between theory and experiments, uncovering novel constitutive relations that describe short crack growth.

Experimentally, we will track the timeseries of all relevant observables: stress, strain, strain-rate and fatigue cycle rate for several loading conditions. The timeseries will be analyzed using well established statistical methods to uncover the underlying constitutive laws.

We aim to perform statistical analysis of short-crack growth experimental and simulation data in order to identify intermittent, avalanche dynamics and possible connections to the “avalanche oscillator” mechanism for plastically deformed metals.
VIDI Career Award (NWO 2013-2018):
How does local relaxational dynamics affect the mechanical response of amorphous complex systems: The hunt for universal features among metals, structural glasses, biological networks and granular systems.

We aim to identify universal effects originating from slow, local, relaxation mechanisms on the mechanical response of amorphous systems, beyond the leading microscopic dynamics. The main target is to identify safe, consistent and experimentally relevant approaches to perform the typically necessary approximation of neglecting local relaxation processes in the dynamical mechanical response of amorphous systems.

Amorphous complex systems are characterized by both the steady-state behaviour and the dynamical conditions under which they were formed. Inexistence of observed order implies that similar-looking configurations may have qualitatively different mechanical responses and the amorphous complexity forces us to consider only the fastest leading dynamics, neglecting all slower dynamical relaxation processes. No matter how slow these may be, they may lead to the collapse of the amorphous rigidity or/and change its nature -- A glass bends, vibrates and responds differently to stress if such slow relaxations are carefully included in simulations. Such slow relaxations are shown crucial to understand microcrystal compression experiments, where the parent crystal is certainly not amorphous, but the dislocation ensemble that drives the deformation is. While swift plastic bursts are driven by dislocation glide processes, slow additional dislocation relaxations (such as climb, cross-slip etc.) lead to a novel self-organized critical state that was labelled as “avalanche oscillator”.

The approach is multi-scale, combining microscopic, semi-coarse-grained and coarse-grained continuum modelling. The approach is also multi-level, with some calculations directed to understand basic questions and fundamental principles while others targeting toward direct comparisons with, typically unpublished, experimental data that are provided by experimentalist collaborators. Finally, the approach is multi-disciplinary, since the pursued ideas are general and widely applicable – we are eager to identify complex systems that may help exploring further the effects of relaxation on the mechanical response of amorphous systems.