

Schedule for the 18th MASM: The Mid-Atlantic Soft Matter Workshop
The University of Pennsylvania, Philadelphia, PA
May 19, 2017

8:40 am

Opening Remarks

8:50 am

Jason Rocks (University of Pennsylvania):
Creating function from disorder in mechanical networks

9:25 am

Arthi Jayaraman (University of Delaware):
Computational design of thermoresponsive soft materials

10:00 am

Soundbite Session I

10:45 am

Coffee Break

11:05 am

Daniel Blair (Georgetown University):
Oobleck revealed! – Microscopic insights into everyone's favorite fluid

11:40 am

Soundbite Session II

12:25 pm

Lunch

1:30 pm

Soundbite Session III

2:15 pm

Coffee Break

2:35 pm

Daniel Ou-Yang (Lehigh University):
Noise and fluctuations in a non-equilibrium and non-linear biological system: what can we learn from them?

3:10 pm

Soundbite Session IV

4:00 pm

Quick Break

4:15 pm

Mehdi Bouzid (Georgetown University):
Aging, stiffening and softening of soft solids

4:50 pm

Zahra Fakhraai (University of Pennsylvania):
Long-Range Correlated Dynamics in Molecular Glasses

5:25 pm

End of Meeting

Jason Rocks, University of Pennsylvania
Creating function from disorder in mechanical networks

Recent advances in metamaterial design have shown that global mechanical properties of disordered spring networks can be tuned by making small changes to the bond structure. Here we extend this idea to tune specific functions into networks. In the simplest case, we tune networks by removing selected bonds to achieve a desired strain between a specified pair of nodes in response to a strain applied to another specified pair of nodes; this strain response constitutes the function that was tuned into the network. We find that creating functions in disordered networks is remarkably easy and typically only requires the modification of a small subset of bonds. These results imply that disordered mechanical networks are highly adaptable - any network can be easily tuned to perform almost any desired function. We also explore the limits of multifunctionality. How many separate independent functions can be simultaneously tuned successfully into a network and how many different targets can be controlled by a single source? We formulate this question as a constraint-satisfaction problem and show the existence of a satisfiability transition in the fraction of successfully tuned networks with mixed first and second order characteristics.

Arthi Jayaraman, The University of Delaware
Computational design of thermoresponsive soft materials

In this talk, I will present my group's recent computational work aimed at understanding thermoresponsive behavior in novel oligonucleic acids (ONAs). Since double stranded DNA (ds-DNA) is the basis of various bio- and nano- technologies, the need for cheaper alternatives and significant synthetic advances have led to the design of DNA mimics with new backbone chemistries (e.g. click nucleic acids, locked nucleic acids). A fundamental understanding of how these backbone modifications in the oligo-nucleic acids impact the hybridization and melting behavior of the double strands is still lacking. We use coarse-grained (CG) and atomistic molecular dynamics simulations along with well-tempered metadynamics calculations to capture the effects of varying backbone chemistries on the H-bonding between complementary nucleobases and the intra-strand base-base stacking, and ONA hybridization/melting. I will also present results on how conjugation of these novel ONAs with biocompatible poly-

mers (e.g. PEG) impacts the melting/hybridization of polymer-conjugated ONA. Our interest in polymer-conjugated ONAs is motivated by their use as building blocks for thermo-responsive gels and networks in biomaterials.

Daniel Blair, Georgetown University
Oobleck revealed! Microscopic insights into everyone's favorite fluid

In this talk I will discuss our recent results on the microscopic physical origins of shear thickening in sheared colloidal suspensions. Using Boundary Stress Microscopy we can resolve the spatial surface stresses in suspensions undergoing continuous thickening. I will present our results on the existence of clearly defined dynamic localized regions of substantially increased stress that appear intermittently at stresses well above the critical stress. With increasing applied stress, these regions occupy an increasing fraction of the system, and that increase accounts quantitatively for the observed shear thickening. The regions represent high viscosity fluid phases appear to share a characteristic size that is determined by the rheometer gap and a viscosity that is nearly independent of shear rate but that increases rapidly with concentration. Remarkably, we find that continuous shear thickening arises from increasingly frequent localized discontinuous transitions between distinct fluid phases with widely differing viscosities.

H. Daniel Ou-Yang, Lehigh University
Noise and fluctuations in a non-equilibrium and non-linear biological system: what can we learn from them?

Mechanical noise and fluctuations are ubiquitous in living biological cells. If we look carefully at small objects inside a living cell, such as organelles or internalized microbeads, we will observe that the positions of these objects are fluctuating incessantly with a magnitude too large to be attributed to thermal motions. We are interested in understanding what may be causing these fluctuations, and what we may learn from them. To answer these questions, we made two key assumptions: 1) the cytoskeleton of living cells is a non-equilibrium mechanical system, containing intracellular molecular motors that consume chemical energy to generate forces and maintain cytoskeletal functions, and 2) the cytoskeleton is a non-linear mechanical network whose shear modulus increases with intracellular stress. We combined the active and passive microrheology methods to measure the

non-thermal fluctuating forces, the mean shear modulus and temporal variation of the mean shear modulus of the cytoskeleton. We found the ratio of the differential shear modulus vs. the differential fluctuating force to be a strongly increasing function of the mean shear modulus. The same trend was found in cells cultured on substrates with different rigidities, and in cells treated with drugs that could alter motor protein activities. Such universal behavior is surprising because the measurements were made at different locations within many different cells. This observation suggests that cells could regulate their mechanical properties by simply making quick and minute adjustments of their intracellular stress instead of taking the slow and energy-expensive processes of polymerizing-depolymerizing their cytoskeleton proteins. *This work was done in collaboration with Steven Ming-Tzo Wei.

Mehdi Bouzid, Georgetown University
Aging, stiffening and softening of soft solids

Disordered elastic solids of soft condensed matter like proteins, colloids or polymers are ubiquitous in nature and important for modern technologies. They can form even at very low solid volume fraction via aggregation into a variety of complex and often poorly connected networks. In most cases, the interaction energies and the size of the aggregating units make these structures quite sensitive to thermal fluctuations, with a rich relaxation dynamics associated to spontaneous local reorganizations often referred to as micro-collapses. Investigating how such different dynamical processes emerge at rest and how they depend on the material microstructure remains a challenge.

We have used 3D numerical simulations of model solids to show that, the relaxation dynamics underlying the aging change dramatically if enthalpic stresses, frozen-in upon solidification are significantly larger than Brownian stresses. The timescales governing stress relaxation respectively through thermal fluctuations and elastic recovery are key: when thermal fluctuations are weak with respect to enthalpic stress heterogeneities, the stress can partially relax through elastically driven fluctuations. Such fluctuations are intermittent, because of strong spatio-temporal correlations that persist well beyond the timescale of experiments or simulations, and the elasticity built into the solid structure controls microscopic displacements, leading to the faster than exponential dynamics reported in experiments and hypothesized by recent theories. Thermal fluctuations, instead, disrupt the spatial distributions of local stresses and their persistence in time, favoring a gradual loss of correlations and a slow evolution of the material properties.

In addition to affecting the time evolution of the material properties at rest, these processes interplay with an imposed mechanical load or deformation and hence may be crucial for the mechanical response of this class of solids. We show how tuning the structural connectivity and the local internal stresses controls the non-linear mechanical response under shear deformations. Our model soft solids exhibit strong localization of tensile stresses that may be released through the breaking of bonds, leading to a strain softening and/or strain hardening. Our findings help to rationalize the non-linear behavior highlighted in various experimental observations.

Zahra Fakhraai, University of Pennsylvania
Long-Range Correlated Dynamics in Molecular Glasses

Nanometer-sized thin films of small organic molecules are widely used in applications ranging from organic photovoltaics and organic light emitting diodes, to protective coatings and high resolution nano-imprint lithography. Physical vapor deposition (PVD) is widely used in manufacturing ultra-thin layers of amorphous organic solids, with an underlying assumption that the properties of these layers are bulk-like. In this presentation, I demonstrate that films of organic glass-formers with thicknesses of 30 nm or less have dynamics significantly enhanced relative to the bulk dynamics at temperatures well below the glass transition temperature, T_g . I show that a sharp glass to liquid transition exists when the thickness of the layer is changed from 40 nm down to 20 nm. This significant change in the glass dynamics is due to the enhanced mobility at the air/glass interface and the length scale over which the effects of this perturbation can propagate due correlated dynamics in the bulk glass. As such, we are able to show that these glassy systems have long-range correlated dynamics over length scales of about ten times the size of the molecules, well exceeding their inter-molecular interaction range. While these measurements are important for a host of applications, they can also help elucidate the fundamental mechanisms of glass transition phenomenon, a question that have attracted numerous theoretical and experimental studies in the past half century. The results of these experiments are directly compared with some of the most well-known models of glass transition.