Program

May 25th, 2012

6th South-East Workshop on Soft Materials

Georgia Tech Physics College of Sciences

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Program

6th Southeast Meeting on Soft Materials Interfaces
Georgia Institute of Technology
Friday, May 25, 2012

Clough Undergraduate Learning Center
AT&T Auditorium 152

Breakfast, Lunch, Breaks: Room 150

8:30 a.m. – 9:00 a.m.
Breakfast and Registration, First Floor.

9:00 a.m. - 9:05 a.m.
Welcome from Alberto Fernandez-Nieves, Georgia Tech

Morning Invited Speaker [Chair: Elisa Riedo]
9:05 a.m. – 9:50 a.m.
David Pine, Key Note Speaker, New York University
From Colloidal Molecules to Colloidal Life: New Directions

9:50 a.m. – 10:00 a.m. Coffee Break

10:00 a.m. – 11:00 a.m.
SOUND BITES I: Colloids, Fluids, Liquid Crystals and Granular Media
[Chair: Victor Breedveld]

Tingnan Zhang, Georgia Tech
A Resistive Force Model for Legged Locomotion on Granular Media
Josefa Guerrero Millan, Georgia Tech
Whipping in Electrified Jets
John Hyatt, Georgia Tech
Internal Structure Changes: Single-Particle Form Factors of Swelling Microgels
Annie Lesiak, Georgia Tech
Calculating States of Phase Coexistence from Computer Stimulations
Jeffrey Gaulding, Georgia Tech
Disulfide Cross-links in Responsive Microgels
Ekapop Pairam, Georgia Tech
Nematic Liquid Crystal Tori
Feifei Qian, Georgia Tech
Walking and Running on Yielding and Fluidizing Ground

Miguel Pelaez-Fernandez, Georgia Tech
On the Equation of State of Soft-particle Suspensions
Nick Gravish, Georgia Tech
Granular Entanglement and the Random Contact Model
Wenbin Mao, Georgia Tech
Continuous Inertial focusing and Separation of Spheroid Particles by Shape
Zachary Mills, Georgia Tech
Using Spiral Structures to Enhance Mixing in Microfluidic Devices
Andrea Scotti, Georgia Tech
Phase Behavior of Soft-particle Suspensions as a Function of Size Polydispersity
Sarah Sharpe, Georgia Tech
Resistance Force in Wet Granular Media
Abiola Shitta, Georgia Tech
Encapsulation of Agrochemicals Via Particle Stabilized Double Emulsions
Joohyung Lee, Georgia Tech
Surfactant-Mediated Electrophoretic Properties of Apolar Dispersions
Jayalakshmi Vallamkondu, Georgia Tech
High-Genus Nematic Liquid Crystal Droplets
Cliff Henderson
Directed Self-Assembly of Block Copolymers

Morning Invited Speaker [Chair: Victor Breedveld]
11:00 a.m. – 11:45 p.m.
Sven Behrens, Georgia Tech
Nano-Scale Roughness of Micron-Sized Particles and its Effect on Particle-Stabilized Emulsions

11:45 p.m. – 1:30 p.m. Lunch & Discussion

Afternoon Invited Speaker [Chair: L. Andrew Lyon]
1:30 p.m. – 2:15 p.m.
Julio Boza, The Coca Cola Company
Innovation and Nutrition Research at the Coca-Cola Company

2:15 p.m. – 3:25 p.m.
SOUND BITES II: Biological Materials, Polymers, Films and Interfaces
[Chair: L. Andrew Lyon]

Jonathan Rubin, Georgia Tech
Hofmeister Effects on Protein Stability
Si Zhou, Georgia Tech
Room Temperature Metastability of Multilayer Graphene Oxide Films
Maeling Tapp, Georgia Tech
Screening for DNA Aptamers for Spherical Gold Nanoparticles

Laura Gray, Emory University
Physical Aging of Polymer Thin Films Stressed During glass Formation
Tung Le, Georgia Tech
Catch-slip transition in DNA Duplex under Shear Stress
Ana West, Emory University
Simulation Grounded, Systematic Approach to Understanding the Long-time Dynamics of Stoichiometrically-mismatched, Self-assembled Protein Networks
Daniel Kovari, Georgia Tech
Biomechanics of Phagocytosis
Suenne Kim, Georgia Tech
Water at Complex Chemical Nano-interfaces
Justin Pye, Emory University
Presence of Free Surface Results in Two Simultaneous Mechanisms Causing Tg Reductions in High Molecular Weight Free-standing Polymer Films
Richard Sullivan, Georgia Tech
Binding of Random DNA Sequences to Gold Nanorods
Eze Ngozi, Georgia Tech
Using Locked Nucleic Acids for Bio-Inspired Colloidal Assembly and Disassembly
Patrick Chang, Georgia Tech
Studying Hyluronan-Dependent Pericellular Matrix Quantitative Particle Exclusion Assays
Annika Kriisa, Emory University
Phase Separation in PS/PVME Blends: the Characterization Via Fluorescence and the Influence of Electrical Fields
Alex Weller, Georgia Tech
Effect of Coating on Nonspecific Cell-particle Association
Chien-Yuan Chang, Georgia Tech
Mechanical Properties of Epitaxial Graphene Oxide
Mónica Fernández-Sierra, Emory University
Effect of Polyamines on the Relaxation of Supercoiled DNA by E. Coli DNA Gyrase
Eilsa Riedo, Georgia Tech
Elasticity of RNA/DNA Molecules
Diane Wiener, Emory University
Transcriptional Regulation: The Role of 186 CI Repressor Protein on Transcription
Yue Ding, Emory University
Effects of Supercoiling and Tension on the Bacteriiophage Lambda Repressor-Mediated DNA Looping

3:25 p.m. – 3:35 p.m. Coffee Break

Afternoon Invited Speaker [Chair: Daniel I. Goldman]
3:35 p.m. – 4:20 p.m.
Carlos Santamarina, Georgia Tech
Particulars of the Particulate: Phenomena in granular materials at the particle/pore-scales

4:20 P.M. Workshop Conclusion

Title and Abstracts

Invited Speakers:

David Pine, Keynote Speaker, New York University

"From Colloidal Molecules to Colloidal Life: New Directions"

We have been developing new colloidal particles with directional, specific interactions with two goals in mind: (1) developing a new colloidal "chemistry" capable of making complex colloidal molecules as building blocks for mesoscopic structures, and (2) creating a process for artificial self-replication. We have demonstrated new colloidal molecules with 2, 3, and 4 fold coordination as well as a colloidal lock-and-key specific interaction similar to idealized models of protein-protein binding.

Sven Behrens, Georgia Tech

"Nano-Scale Roughness of Micron-Sized Particles and its Effect on Particle-Stabilized Emulsions"

Adriana San Miguel and Sven H. Behrens, School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Colloidal particles can strongly adsorb to liquid interfaces and stabilize emulsions against droplet coalescence, the effectiveness of which depends crucially on the particle wettability. From the study of macroscopic solids, surface wetting is known to be influenced strongly by nano-scale roughness (as seen *e.g.* in the "Lotus effect" or in anti-fog coatings); similarly, strong effects of particle roughness on particle-stabilized emulsions should be expected. Here we report the first experimental study of particle wetting and particle-mediated emulsion stability in which particle roughness could be varied continuously without varying the surface chemistry. We demonstrate an enabling method for preparing particles and macroscopic substrates with tunable nano-roughness and correlate the extent of roughness quantitatively with surface wetting (measured *via* the three-phase contact angle) and with emulsion stability (quantifiable *via* the maximum capillary pressure). Our results confirm a dramatic influence of roughness on wetting, emulsion stability, and even the type of emulsion formed (o/w vs. w/o) upon mixing oil with an aqueous particle dispersion. Whether particle roughness benefits emulsion stability or not is seen to depend on both the size and shape of the surface features.

Julio Boza, The Coca-Cola Company

"Innovation and Nutrition Research at The Coca-Cola Company"

An overview about the Coke innovation activities in different fields such as Packaging, Processing, Sustainability, Environment, Product Portfolio, Research, especially focused on the research efforts made in the scientific substantiation of nutrition and health related effects of functional juice products.

Carlos Santamarina, Georgia Tech

"Particulars of the Particulate: Phenomena in granular materials at the particle/pore-scales"

The complex nature of granular materials and their intricate behavior in the context of engineering applications remain challenging after a century of extensive scientific research and engineering advances. Fascinating underlying phenomena and processes are revealed as selected examples of coupled thermo-hydro-bio-chemo-mechanical processes that take place in granular materials are analyzed at the particle/pore scales.

Sound Bites I: Colloids, Fluids, Liquid Crystals and Granular Media

Tingnan Zhang, Georgia Tech

"A Resistive Force Model for Legged Locomotion on Granular Media"

Understanding the mechanics of legged locomotion on granular media is challenging because no comprehensive force models yet exist to describe the forces during localized intrusion into granular media. While recent studies have modeled the lift and drag forces on animal limbs by simple one-dimensional force laws such as the vertical penetration force or horizontal drag force on a plate moving in granular media, it remains difficult to accurately model forces on limbs of complex geometries moving within granular media along complex trajectories. To address this problem, we develop a two-dimensional resistive force model in the vertical plane, by dividing an intruder of complex morphology and kinematics, e.g., a robot's c-leg rotated through granular media (~ 1 mm diameter poppy seeds), into small segments, and measuring segmental forces as a function of angle of attack, direction of motion, and depth. Both segmental lift and drag increase approximately proportionally with depth, and depend sensitively on angle of attack and direction of motion due to symmetry breaking by gravity. Summation of segmental forces over the intruder predicts the net forces on both c-leg and reversed c-leg rotated through granular media. The resistive force model is valid at low speeds (< 0.5 m/s) when the inertia of the grains is negligible and the granular material behaves like a "frictional fluid". The combination of the resistive force model with a multi-body dynamic simulator (MBDyn) accurately predicts the speeds of a small legged robot (15 cm, 150 g) moving on granular media using both c-legs and reversed c-legs.

Josefa Guerrero Millan, Georgia Tech

"Wipping in Electrified Jets"

Whipping is a non-axysymmetric instability exhibited by electrified jets, which usually manifests in a chaotic fashion. As a result, its structure and properties are difficult to quantify experimentally. We use electro-coflow as a way to generate a well defined whipping structure and show (i) it is helicoidal and (ii) has a phase velocity that depends of its geometry and on the charge carried by the whipping jet.

John Hayatt, Georgia Tech

"Internal Structure Changes: Single-Particle Form Factors of Swelling Microgels"

We study the microscopic, internal structure changes of microgels using static light scattering. These microgels are pNIPAM copolymerized with acrylic acid and therefore swell at lower temperatures and higher pH. The microgel form factors for the deswollen case are well-described by a soft-sphere model, however at higher swollenness the microgel structure opens up and they begin to more closely resemble large star polymers.

Annie Lesiak, Georgia Tech

"Calculating States of Phase Coexistence From Computer Stimulations"

We present a novel method to calculate states of phase coexistence from computer simulations. Our method relies on microcanonical molecular dynamics simulations of condensed matter systems described through the use of classical force fields. To estimate states of phase coexistence, we simulate the quasi-static heating process of the crystal, we derive a numerical equation of state, and we finally apply a Maxwell equal-area construction to separate the regions of equilibrium and non-equilibrium. This method is tested on the hard-sphere model.

Jeffrey Gaulding, Georgia Tech
"Disulfide Cross-links in Responsive Microgels"
Colloidal hydrogel particles, or microgels, are of great interest for drug delivery applications, due to their biocompatible nature, high loading capacity, and chemical versatility. Rational design of delivery vehicles relies heavily on the application of tools that allow control over microparticle chemical functionality and architecture. In particular, the ability to use orthogonal coupling chemistries enables more robust post-synthetic particle modifications, such as allowing the incorporation of both a targeting ligand and a therapeutic load. One such tool, precipitation polymerization, has been demonstrated as a versatile means to make a variety of microgel compositions. However, it is typically incompatible with thiol-chemistry, due to potential side reactions during the polymerization. Thiols offer access to an attractive series of very selective conjugation reactions that require mild conditions. We have recently demonstrated synthetic techniques that enable the incorporation of intact disulfide bonds within thermo-responsive microgel particles using aqueous precipitation polymerization. The presence of a second non-degradable cross-linker during the synthesis enables the formation of redox-responsive microgels; particles capable of network swelling and expression of reactive thiols for particle assembly or bioconjugation. The introduction of thiol-functionality within a microgel is an enabling step towards further development of complex drug delivery architectures, and present opportunities for multiple-orthogonal chemical functionalization through combination with other established synthetic techniques.

Ekapop Pairam, Georgia Tech
"Nematic Liquid Crystal Tori"
We generate stable and toroidal nematic liquid crystal droplets inside viscoelastic media. We look at these droplets between crossed-polarizers and find organizational changes as a function of the aspect ratio.

Feifei Qian, Georgia Tech
"Walking and Running on Yielding and Fluidizing Ground"
A recently developed small, lightweight (10 cm, 25 g) bio-inspired hexapedal robot, dynaRoACH, can move on a granular substrate (closely packed 3 mm diameter glass particles) at speeds up to 50 cm/s (5 body length/s), approaching the locomotor performance of a small, high-performing, desert-dwelling lizard on granular surfaces. To reveal how the robot achieves this high performance, we used high speed imaging to capture kinematics, and developed a numerical multi-body simulation of the robot coupled to an experimentally validated discrete element method (DEM) simulation of the granular media. Average forward speeds measured in both experiment and simulation agreed well, and increased non-linearly with stride frequency, reflecting a change in the mode of propulsion. At low frequencies, the robot used a quasi-static "rotary walking" mode, in which the granular material yielded as the legs penetrated and then solidified once vertical force balance was achieved. At high frequencies, duty factor decreased below 0.5 and aerial phases occurred. The propulsion mechanism was qualitatively different: the robot ran rapidly by utilizing the speed-dependent fluid-like inertial response of the material. We used the simulation to vary granular particle friction that was inconvenient to vary in experiment to test performance and reveal limits of stability of the robot. In addition to advancing the design and modeling of small platforms on complex terrain, our studies reveal that such small robots are physical models to study how small animals achieve high performance on granular substrates.

Miguel Pelaex-Fernandez, Georgia Tech

"On the Equation of State of Soft-particle Suspensions"

We measure the osmotic pressure and the packing fraction of suspensions comprised of microgel particles. We do this as a function of individual-microgel stiffness. These experiments thus directly provide the equation of state for these suspensions and how it depends on the mechanical properties of individual particles.

Nick Gravish, Georgia Tech

"Granular Entanglement and the Random Contact Model"

Granular media with grains of sufficiently complex geometry, such as u-shaped particles, entangle with neighboring particles. Piles formed from these geometrically cohesive particles may be strengthened by such inter-particle entanglement. We previously studied the relaxation of free-standing vertical columns formed from u-shaped particles of barb length, l, and constant width, w, to determine how bulk strength is affected by particle geometry. We found that particle ensembles with intermediate barb length $l/w=0.375$ displayed the longest relaxation times and we hypothesized that this optimum particle shape is a result optimum particle entanglement in the bulk. In this study we employ a monte-carlo simulation of particle packing and the random contact model to study the packing statistics of concave particles. The random contact model states that the volume fraction, phi, of particles distributed at random is related to the particle volume v_p, excluded volume v_e, and the average number of contacts C, by $phi = Cfrac{v_p}{v_e}$. Volume fraction measurements obtained in simulation and experiment are in good agreement and the random contact model fits the data well for a constant $C = 8.74$. In simulation we measure the density of particle entanglements, rho_{ent} and find that rho_{ent} is maximum at $l/w = 0.394$ near the observed maximum in experiment. The random contact model explains this maximum as a competition between particle packing which decreases monotonically with $l/$ and particle entanglements which increases monotonically with l/w.

Wenbin Mao, Georgia Tech

"Continuous Inertial Focusing and Separation of Spheroid Particles by Shape"

An approach to separate shaped-particles can be used to isolate disease-causing cells for diagnostics or can aid in purifying non-spherical targets in applications ranging from food science to drug delivery. We use a hybrid numerical method that combine the lattice Boltzmann model and lattice spring model to investigate the dynamics of neutrally buoyant spheroid particles in a Poiseuille flow. Particle rotation in a plane perpendicular to the vortex direction is found to be a necessary component in producing different equilibrium positions that depend on particle rotational diameter. These differences are large enough to enable high-purity, continuous, passive and high-throughput shape-based separation downstream.

Zachary Mills, Georgia Tech

"Using Spiral Structures to Enhance Mixing in Micorfluidic Devices"

We are using three dimensional computer simulations to examine mixing in a microchannel which encompasses a periodic array of spiral structures. The channel is filled with a viscous fluid and tracer particles are used to quantify the mixing that is induced by the structures. To model the system, we are employing the lattice Boltzmann model coupled with the lattice spring model. We plan to investigate how spiral structures can influence the mixing rates by varying the dimensions and the spacing between each spiral. From these simulations, we can determine the size and spacing of spiral structures that will optimize mixing in microfluidic devices.

Andrea Scotti, Georgia Tech

"Phase Behavior of Soft-particle Suspensions as a Function of Size Polydispersity"

It is well known that polydispersity suppresses crystallization in hard spheres systems. Our aim is to investigate and understand how size polydispersity affects the phase behavior of soft-sphere suspensions based on PNIPAM microgels. We create samples with increased polydispersities from families of monodisperse suspensions and study the phase behavior as a function of volume fraction.

Sarah Sharpe, Georgia Tech

"Resistance Force in Wet Granular Media"

Wet granular media such as soil and beach sand are abundant in nature. Numerous animals live on and within these soils and must cope with resistance forces which vary depending on wetness and compaction. Repeatable homogenous preparations of wet granular media (GM) are created by using a sieve apparatus; the wet substrate is loaded into a top container separated from the bottom container by a mesh grid (3 mm spacing). The media falls through as a result of vertical agitation and creates a loosely packed state without large voids. Empirical drag measurements in wet GM of 0.3 mm glass particles prepared into a loosely packed state revealed that resistance force increased by a factor of three as water content (W, the mass of water/mass of GM) increased to 3%, after which force became approximately independent of W. Further, resistance force in a LP dry GM state was approximately constant while force in wet GM oscillated during movement.

Abiola Shitta, Georgia Tech

"Encapsulation of Agrochemicals via Particle Stabilized Double Emulsions"

Aqueous formulations of crop protection agents such as fungicides and insecticides often contain additives ("adjuvants") that facilitate uptake by the plants, but can also reduce the stability and efficacy of the active ingredient. In this project we aim at minimizing such undesired side effects by physically separating the active ingredient from the adjuvant via microencapsulation. Specifically, we are using water-in-oil-in-water (w/o/w) double emulsion droplets as templates in the capsule assembly and utilize the concept of particle-assisted spreading, familiar from oil films on a macroscopic water surface, to ensure a minimum thickness of the oil film in w/o/w droplets and of the capsules templated by these droplets.

Joohyung Lee, Georgia Tech

"Surfactant-Mediated Electrophoretic Properties of Apolar Dispersions"

It has long been known that charge control agents (surfactants) can lead to a dramatic increase in electric conductivity and to particle charging in nonpolar liquids, which are often considered to be charge-free because of large energetic costs for separating oppositely charged ions. Electric charging in nonpolar liquids can be applied in a wide range of applications, such as the prevention of explosion hazards in petroleum handling, the design of electrophoretic displays, liquids toners, drug delivery systems, the development of detergents, or in the study of new types of crystalline materials. Despite its huge potential applicability, the mechanism of surfactant-mediated charging in nonpolar liquids is not well understood. In the Behrens research group, we have found that even nonionic surfactants can promote electric charging in these charge-hostile media, and in some cases do so more efficiently than ionic surfactants. Our preliminary results indicate that particle charging in nonpolar oils can proceed through a variety of different mechanisms, which have yet to be fully disentangled. We are now attempting to synthesize and characterize home-made surfactants under systematic variation of the most relevant system parameters, such as the size of the polar headgroup, the presence of ionizable moieties, or the acid-base properties of the surfactants molecules. The study is performed in close collaboration with Hewlett-Packard, who will directly apply our joint insights to the next generation of color reflective displays.

Jayalakshmi Vallamkondu, Georgia Tech

"High-Genus Nematic Liquid Crystal Droplets"

We will discuss the defect structures that originate in nematic droplets with two or more handles. In these cases, the topology of the bounding surface requires the presence of defects. Our experiments elucidate where do these defects locate and how many of them populated the ground state of the system.

Cliff Henderson

"Directed Self-Assembly of Block Copolymers"

Current tools and material technologies for nanoscale patterning by traditional single layer lithographic techniques have reached their practical limit at feature pitches on the order of 80 nm. For industrial manufacturing of smaller feature pitches to continue in fields such a integrated circuits, alternative nanopatterning technologies will be needed. The use of self-assembly of block copolymers on lithographically patterned template surfaces, referred to commonly as directed self-assembly (DSA) of block copolymers, is one promising technology that may be able to meet these challenges of producing smaller feature pitches and sizes while utilizing and extending current lithographic technologies. Our work in this area has been directed at two main goals: (1) experimentally developing high X polymers, guiding layers, and processes to achieve sub-20 nm pitch DSA and (2) developing and utilizing simulation tools to understand the fundamental polymer physics, material properties, and process factors that control the behavior in such systems. A quick overview of achievements in high X polymers (e.g. PS-b-PAA and PS-b-PHOST) that can produce sub-20 nm pitch patterns will be given and an overview of fundamental learning gained about structure-process-property relations from our detailed molecular dynamics simulation work will be given.

Sound Bites II: Biological Materials, Polymers, Films and Interfaces

Jonathan Rubin, Georgia Tech

"Hofmeister Effects on Protein Stability"

Ion-specific (Hofmeister) effects strongly influence protein physical stability. This work studies two manifestations of these effects in pharmaceutical formulations of proteins and in amyloid diseases.

Si Zhou, Georgia Tech

"Room Temperature Metastability of Multilayer Graphene Oxide Films"

Multilayer graphene oxide (GO) is a material holding great promise in future energy storage and nano-electronic technologies. This material remains qualitatively known to date. In this work, we present a combined experimental X-ray photo-emission spectroscopy and density functional theory study of the structural, chemical, and thermal stability of multilayer GO grown epitaxially on silicon carbide. This investigation shows that at room temperature multilayer GO is a metastable material. GO films undergo spontaneous modifications and chemical reduction with a relaxation time of about one month. Our study suggests that the presence of excess H chemisorbed on the oxidized graphene sheets in GO is at the origin of the metastable character of multilayer GO. These H species favor the reduction of epoxide groups and the consequent transformation of hydroxyls into water molecules intercalated between the graphene layers.

Maeling Tapp, Georgia Tech

"Screening for DNA Aptamers for Spherical Gold Nanoparticles"

Aptamers are single-stranded oligonucleotide sequences that exhibit high affinity and high specificity binding for nonnucleotide targets. Using a procedure called "systematic evolution of ligands by exponential enrichment" (SELEX), aptamers can be identified from combinatorial libraries consisting of random sequences. This in vitro selection procedure has led to the discovery of aptamers for a variety of targets including but not limited to ions, small macromolecules, and whole cells. Due to their small molecular weight, ease of processing, and long-term stability, aptamers are now increasingly explored as potential alternatives to antibodies as high affinity ligands. These characteristics highlight the potential impact of aptamers in areas such as biosensing, diagnostics, and therapeutics. Gold nanoparticles have been widely studied for various diagnostic, imaging and therapeutic applications due to their shape and size-dependent optical properties. Tight control over the size distribution and shape of gold nanoparticles using conventional solution precipitation approaches, however, is challenging. In addition, subsequent assembly of nanoparticles into well-organized spatial patterns on substrates can pose additional challenges. The overall goal of the proposed research is to identify aptamer sequences from a random library that bind both to gold nanoparticles and to gold ions. If successful, this approach to aptamer screening will potentially allow for the simultaneous precipitation and patterning of homogeneous, spherical gold nanoparticles.

Laura Gray, Emory University

"Physical Aging of Polymer Thin Films Stressed During glass Formation"

How stress and mechanical deformation impart mobility to glasses and jammed materials is an area of common interest from granular materials to polymers. These studies have been primarily on materials where the glassy state was formed stress free. Here, we investigate the stability of polymer glasses where stress is applied during the formation of the glassy state (thermal quench). We hypothesize that different stresses may trap the glassy state into different potential energy minima, dictating the subsequent physical aging rate of the material. Ellipsometry measures the physical aging rate of polystyrene films transferred onto silicon by quantifying the time-dependent decrease in film thickness that results from the increase in average film density during aging. We have constructed a unique jig to apply a known stress to free-standing films during the thermal quench. Our results may explain the faster aging behavior seen in gas separation membranes with decreasing thickness.

Tung Le, Georgia Tech

"Catch-slip Transition in DNA Duplex Under Shear Stress"

DNA experiences a wide range of mechanical stress in cells. Structural transitions of DNA under mechanical stress has thus been a subject of intensive study. One interesting counter-intuitive finding is that double-stranded DNA overwinds under small tensile forces, thus becoming energetically more stable. This phenomenon bears some similarity to the catch bond mechanism where the lifetime of an adhesion bond becomes longer under tension. To investigate whether DNA strand separation can exhibit a catch bond like behavior, we measured the stability of a duplex DNA in a loop geometry using single-molecule FRET. In this scheme, bending elasticity of the looped DNA exerts ~piconewton shear force on the short duplex, and the shear force can be changed by changing the loop size. Surprisingly, we observed that separation of a 10-bp duplex occurred more slowly with increasing force, reminiscent of a catch bond. In contrast, a 7-bp duplex became more unstable with increasing force, indicative of a normal slip bond. To the best of our knowledge, this is the first time that a catch-slip transition has been observed in DNA strand separation.

Ana West, Emory University

"Simulation grounded, Systematic Approach to Understanding the Long-time Dynamics of Stoichiometrically-mismatched, Self-assembled Protein Networks"

We present mesoscale simulation results and analytical derivations for the long-time equilibrium dynamics of model peptide networks assembled from mixing stoichiometrically mismatched amounts of "junctions" and "linkers" components. The analysis evaluates how the migration of defects controls the rate of relaxation of shear stress, and how this rate is related to junction multiplicity, defect concentration, linker stiffness, single vs. multiple junction pairings, and linker looping ability. The shear-relaxation time and viscosity are predicted to fall away sharply when junction and linker concentrations are mismatched by even 1%. The mean stress relaxation per defect migration event obtained through simulations of low valent networks with single junction pairings is from two to three times greater than assumed by standard simple theories. The rates of defect migration in networks with multiple junction pairings and/or loops are accelerated and result in lower shear relaxation times. Discounting the looped linkers from the density of active chains and treating linkers involved in multiple junction pairings as parallel springs leads to a static shear modulus (G) linear in the number of effective elastic chains (NL). Furthermore, the time-dependence of viscosity during gel "aging" is modeled as an approach to equilibrium through diffusion-limited recombination of complementary defects.

Daniel Kovari, Georgia Tech

"Biomechanics of Phagocytosis"

Phagocytosis is the process by which cell uptake large foreign bodies. It is one of the main methods by which white blood cells work to suppress pathogens. Physical changes in the cell include rearrangement and polymerization of actin in the phagocytic cup, large membrane deformations, increased membrane area via exocytosis, and closure of the phagocytic cup through membrane fusion. Hence, phagocytosis is a fine-tuned balance between biophysical cellular events and chemical signaling, which are responsible for driving these materials and mechanical changes. We present a series of assays designed to probe the physical/mechanical parameters that govern a cell during phagocytosis.

Suenne Kim, Georgia Tech

"Water at Complex Chemical Nano-interfaces"

Abstract: The understanding and the ability to manipulate fluids at the nanoscale is a matter of continuously growing scientific and technological interest. Fluid flow in nano-confined geometries is relevant for biology, polymer science and geophysics. Here, we present experiments which show how the boundary viscosity of water strongly depends on the wetting properties of the confining surfaces. This dependency is fully explained by considering water slippage at a stationary solid surface. Furthermore, we modify the surface chemistry of a polymer film at the nanoscale by using ThermoChemical NanoLithography (TCNL) to study water at the interface with chemical nanopatterns with hydrophobic/hydrophilic adjacent regions.

Justin Pye, Emory University

"Presence of Free Surface Results in Two Simultaneous Mechanisms Causing Tg Reductions in High Molecular Weight Free-standing Polymer Films"

Boundary effects have been seen to affect glassy dynamics across a variety of confined systems including colloids, polymers, and small molecules. The presence of a free surface is known to cause reductions in the glass transition temperature (Tg) in thin polymer films, but the fundamental mechanism causing this phenomenon is still unknown. Our recent measurements have demonstrated the presence of two separate mechanisms simultaneously causing Tg reductions in high molecular weight (MW) free-standing polymer films. We have observed two distinct reduced Tgs within single high MW free-standing polystyrene films demonstrating the presence of a MW independent and a MW dependent mechanism. We believe the MW independent mechanism is common across polymers, small molecules, and colloids. The characteristics of these two mechanisms and their manifestation in thin polymer films will be discussed.

Richard Sullivan, Georgia Tech

"Binding of Random DNA Sequences to Gold Nanorods"

Gold nanorod synthesis typically requires cetyltrimethylammonium bromide (CTAB) to form a stabilizing bilayer the nanorod surface. We have explored displacing this CTAB layer with DNA strands from a random sequence library during nanorod growth. UV-vis results indicate that the addition of DNA to gold seed during nanoparticle formation resulted in a significant shift of the longitudinal peak wavelength. TEM confirmed that these spectral differences stemmed from the formation of nanospheres and nanorods of varying size and aspect ratio, depending the DNA sequences characteristics such as base length and secondary structure (single-stranded vs double-stranded).

Eze Ngozi, Georgia Tech

"Using Locked Nucleic Acids for Bio-Inspired Colloidal Assembly and Disassembly"

Oligonucleotides hold great promise as a programmable biomaterials assembly and disassembly tool. Modified oligonucleotides, such as locked nucleic acid (LNA), have been of recent interest in physiological applications due to their superior nuclease resistance over DNA; LNA is promising due to its reportedly low cytotoxicity effects. Here, we focus on programming the isothermal assembly and disassembly of LNA-linked colloidal particles. Initially, to drive LNA-mediated particle assembly, we employ 9-base-long duplexes that are either 1) perfectly matched or 2) contain a single, center mismatch. Then, to drive LNA-mediated disassembly, 15-base-long, perfectly matched target strands are added to the suspension. Fluorescence-based confocal microscopy confirms substantial assembly for both perfectly matched and mismatched cases. Flow cytometry results indicate that the perfectly matched targets are more efficient at displacing the mismatched duplex strands than perfectly matched duplex strands. This work demonstrates that LNA can be used to assemble and disassemble colloidal particles under isothermal and physiologically relevant conditions.

Patrick Chang, Georgia Tech

"Studying Hyaluronan-Dependent Pericellular Matrix Quantitative Particle Exclusion Assays"

The pericellular coat is a grafted polymer matrix on the surface of many cell types including fibroblasts, chondrocytes, epithelial and smooth muscle cells. This highly-hydrated matrix is invisible in the microscope, yet can extend 1-20 microns out from the cell surface. The thickness of the cell coat as well as its non-uniform spatial organization correlates directly with cell mitosis as well as with cell migration. Its presence has also been associated with cancer metastasis. The structure and mechanical properties of the cell coat are suspected to help cells regulate their adhesion to the surrounding matrix, facilitating cell proliferation and migration – both which rely on a complex regulation of the cell's anchorage to the substrate. Yet to date, tools to characterize the physical properties of the cell coat have been lacking and this hypothesis has not been validated. Nevertheless, upregulating or down regulating cell coat thickness is a therapeutic approach in helping with wound healing, and one being considered to possibly diminish the spread of cancer. Our studies aim to characterize the molecular organization (i.e. the ultrastructure) of the cell coat for the first time using a suite of biophysical techniques ranging from quantitative particle exclusion assays, optical force probe microscopy, and fluorescence recovery after photobleaching (FRAP). Here, our results from quantitative particle exclusion assays are presented. The distribution of passivated microparticles (40, 200nm diameter) within the cell coat are analyzed. Assuming thermal and diffusive equilibrium, this distribution can be related to the chemical potential of the microspheres and the potential of the polymer matrix. Extracting the potential in the cell coat, in turn, yields a prediction of the correlation length or equivalently the mesh size of the cell coat versus distance to the cell surface.

Annika Kriisa, Emory University

"Phase Separation in PS/PVME Blends: the Characterization via Fluorescence and the Influence of Electrical Fields"

We present the results of thermally induced phase separation in polystyrene (PS) / poly(vinylmethylether) (PVME) blends using fluorescence emission of pyrene and anthracene dyes covalently bonded to the PS component. We observe sharp increase in fluorescence intensity upon phase separation for all fluorophores with little change in spectral shape. Fluorophores in which the dye is located closer to the PS backbone show phase separation earlier than the fluorophores in which the dye is located further away on covalent tether. We are currently studying the electrical field influence on the miscibility of PS/PVME blends. Recently, the origin of miscibility in PS/PVME blends was identified to be the presence of weak hydrogen bonds between blend components. We believe the electrical fields capable of breaking those weak hydrogen bonds and causing considerable drop in the lower critical solution temperature (LCST) phase diagram.

Alex Weller, Georgia Tech

"Effect of Coating on Nonspecific Cell-particle Association"

Nonspecific binding of drug carriers to cells can lead to undesirable cytotoxicity effects on normal cells as well as reduce the overall therapeutic index of injected pharmaceuticals. To minimize nonspecific binding, polymeric coatings are often included on drug carriers. We are exploring a triblock PEG-PPG-PEG called Pluronic F-108 as a stealth coating on model 200 nm fluorescent drug carriers. Using flow cytometry, we find that nonspecific binding of fluorescent nanoparticles to C6 rat glioma cells is significantly reduced by a Pluronic coating.

Chien-Yuan Chang, Georgia Tech

"Mechanical Properties of Epitaxial Graphene Oxide"

The Mechanical properties of reduced epitaxial Graphene Oxide are investigated here by atomic force microscopy(AFM). In order to measure the mechanical properties of the epitaxial graphene as a function of the annealing temperature, we employ modulated the nano-indentation method in situ with thermal treatments in controlled temperature.

Mónica Fernández-Sierra, Emory University

'Effect of Polyamines on the Relaxation of Supercoiled DNA by E. Coli DNA Gyrase"

Polyamines are small polycationic molecules involved in numerous essential cellular processes. Polyamines, such as spermidine, can bind to DNA and electrostatically increase its flexibility by decreasing the repulsion between negative charges on the phosphate backbone. Elevated polyamine concentrations are found in cancerous tissues and inhibition of their synthesis prevents cell growth. Thus, there is much interest in understanding the roles of polyamines in cancer. Due to their effect on DNA structure, polyamines can modulate the activity of enzymes that maintain DNA topology, such as topoisomerases, which are essential in DNA metabolism and required for cell viability. This makes topoisomerases an important target for cancer therapies. In order to characterize the effects of polyamines on the activity of DNA gyrase, a type-II topoisomerase, we employed Magnetic Tweezers, a single-molecule DNA manipulation technique which enables us to control the level of supercoiling on DNA molecules and to detect the action of individual enzymes on supercoiled DNA. We hypothesize that changes in polyamine concentration can modulate the activity of type-II topoisomerases by shifting the topological equilibrium between twisted and supercoiled DNA. The E. coli DNA gyrase relaxes supercoils at a rate of 2 turns/s, seldomly pausing and removing 4-10 turns per reaction burst. In the presence of 2.4mM spermidine, gyrase relaxed supercoils with rates comparable to those reached in the absence of polyamine. However, spermidine caused gyrase to pause frequently, relaxing only an average of 2 turns in each relaxation burst. Pauses in the presence of spermidine are three times shorter than the few ones observed without polyamine. A better understanding of the synergy between polyamines and topoisomerases may indicate new specific ways to interfere with cancerous cell proliferation.

Eilsa Riedo, Georgia Tech

"Elasticity of RNA/DNA Molecules"

It is well known that the presence of ribonucleotides (rNMPs) in DNA can cause DNA backbone distortion and might alter the mechanical properties of DNA. The presence of a single ribonucleotide in DNA could alter the function of DNA replication and transcription, the interaction of DNA with histone proteins, or it could interfere with the process of gene silencing. Thus, understanding how the mechanical properties of DNA are modified by the presence of embedded single ribonucleotides can help to elucidate the consequences of this modified nucleic acid structure. This project is at the interface between the fields of chemistry, physics and biology and it is a collaborative effort between Riedo's group and Storici's group.

Diane Wiener, Emory University

"Transcriptional Regulation: The Role of 186 CI Repressor Protein on Transcription"

Transcription of DNA to RNA is a central location for regulation of gene expression. Among the numerous methods of regulation, two include the repression of gene expression by repressor proteins and transcriptional interference by other transcription processes. Bacteriophage 186 is an excellent model system to probe both of these modes of transcriptional regulation. Coliphage 186, like bacteriophage λ, maintains a lytic and lysogenic reproductive pathway. However, unlike bacteriophage λ, the two RNA polymerase promoters for the lytic and lysogenic switch are convergent. The lytic and lysogenic pathways are regulated by the repressor protein 186 CI. 186 CI forms a 14-mer arranged in a wheel, where the N-terminal domain preferentially binds to several specific DNA operator sites, looping and even wrapping the DNA around the 186 CI wheel, thereby preventing transcription at the strong lytic promoter site. Further, the 186 CI protein may also interact with the E. coli RNA polymerase, influencing the transcriptional interference between the two convergent lytic and lysogenic promoters. Here, we present preliminary single-molecule magnetic trapping measurements of the binding, looping, and wrapping dynamics of the 186 CI protein to the specific operator sites. Additionally, atomic force microscopy images are quantified to observe the influence of the 186 CI protein looped or wrapped state on a transcribing E. coli RNA polymerase. Characterization of transcriptional regulation in coliphage 186 provides insight into gene regulation with potential implication to histones where by DNA is wrapped twice about the histone octamer, similar to the wrapping of DNA about the 186 CI wheel.

Yue Ding, Emory University

"Effects of Supercoiling and Tension on the Bacteriiophage Lambda Repressor-Mediated DNA Looping"

Protein-mediated DNA looping is widely found as a topological regulatory mechanism in DNA transcription and other genetic process in vivo. The loop formation probability is mainly regulated by the loop size, protein concentration, supercoiling level of the genomic DNA, and local tension generated from the action of motor protein and enzymes. The supercoiling level varies at different times in cell cycle and likely at different locations in the genome, and a change of the local negative supercoiling level has been known to affect gene expression and regulation. However, little is known about the dynamics of how supercoiling and enzyme-generated tension control gene regulation by affecting DNA looping probability and stability. We present single molecule measurements to study the effects of supercoiling and tension on a loop induced by the lambda repressor (CI protein) binding to two regions of specific sites in bacteriophage lambda DNA. The loop helps keeping the concentration of the repressor at the appropriate level to maintain the quiescent state, while guaranteeing efficient switching to virulence if necessary. Though even the lowest force prevents the wild type 2317 bp-long loop formation in vitro, the formation and breakdown of a 1051bp-long loop was observed under <1pN tension in unwound DNA at physiological CI concentrations. Furthermore, negative supercoiling stabilized the loop against increased tension, in agreement with our previous observation on a 400bp-long loop. The effect of DNA supercoiling on the formation and breakdown of different size loops is important for the quantitative understanding of the physiological role that DNA supercoiling and tension may have on loop-based gene regulation. Since the genome supercoiling level depends on the energy level and health status of a cell, our investigation sheds light on the dependence of some regulatory mechanisms on these two factors.