2006 APS March Meeting Baltimore, MD http://www.aps.org/meet/MAR06

#### Monday, March 13, 2006 8:00AM - 11:00AM – Session A8 DFD GSNP: Pattern Formation and Nonlinear Dynamics Baltimore Convention Center 314

8:00AM A8.00001 The effects of initial seed size and transients on dendritic crystal growth ANDREW DOUGHERTY, THOMAS NUNNALLY, Dept. of Physics, Lafayette College — The transient behavior of growing dendritic crystals can be quite complex, as a growing tip interacts with a sidebranch structure set up under an earlier set of conditions. In this work, we report on two observations of transient growth of NH<sub>4</sub>Cl dendrites in aqueous solution. First, we study growth from initial nearly-spherical seeds. We have developed a technique to initiate growth from a well-characterized initial seed. We find that the approach to steady state is similar for both large and small seeds, in contrast to the simulation findings of Steinbach, Diepers, and Beckermann[1]. Second, we study the growth of a dendrite subject to rapid changes in temperature. We vary the dimensionless supersaturation  $\Delta$  and monitor the tip speed v and curvature  $\rho$ . During the transient, the tip shape is noticeably distorted from the steady-state shape, and there is considerable uncertainty in the determination of the curvature of that distorted shape. Nevertheless, it appears that the "selection parameter"  $\sigma^* = 2d_0 D/v \rho^2$ 

#### 8:12AM A8.00002 Control of eutectic solidification microstructures through laser spot pertur-

remains approximately constant throughout the transient. [1] I. Steinbach, H.-J. Diepers, and C. Beckermann, J. Cryst. Growth, 275, 624-638 (2005).

**bations**, SILVERE AKAMATSU, CNRS, KYUYONG LEE, Ames Laboratory, WOLFGANG LOSERT, UMD — We report on a new experimental technique for controlling lamellar eutectic microstructures and testing their stability in directional solidification (solidification at fixed rate V in a uniaxial temperature gradient) in thin sample of a model transparent alloy. A eutectic binary alloy solidifies into a mixture of two crystal phases. In stationary regimes, periodic front patterns made of an alternate stacking of lamellae of the two solid phases are observed. We observe the solidification front in real time by optical microscopy. We use micromanipulation with laser spot arrays for perturbing the solidification front on a scale ranging from one to ten times the average value of the lamellar spacing (spatial period), i.e., typically 10 to 100 microns. These perturbations arise from local heating due to the absorption of the laser light by the liquid slightly ahead of the front. We use the laser spot perturbation technique as a tool for mapping out the large range of accessible lamellar spacings at given V and for creating desired patterns (smooth spatial modulation, tilt domains).

#### 8:24AM A8.00003 Pattern Formation in a NaCl Crystal undergoing Strain-enhanced Dissolu-

tion, ZVI KARCZ, DENIZ ERTAS, RICHARD POLIZZOTTI, ExxonMobil Research and Engineering, EINAT AHARONOV, Weizmann Institute of Science, CHRIS SCHOLZ, Lamont Doherty Earth Observatory — Observations of an initially circular contact (~300 $\mu$ m in diameter) between the [100] face of a single-crystal NaCl shaped as a truncated cone and a flat silicate plate immersed in saturated solution indicate that the crystal deforms in two sequential stages under constant normal load. The first is characterized by contact area reduction and slow convergence rates, and the second by fluctuations in contact area and fast and fluctuating convergence rates. Fluctuations are on a timescale of ~14 hours. The transition between the stages occurs at the maximum contact stress, which shortly precedes the maximum convergence rate. Confocal images indicate that the crystal dissolves coaxially during the first stage, producing a decreasing static contact. During the second stage, the contact shape is highly irregular, with channels and ridges forming inside the contact. These observations reflect a system evolving towards a non-equilibrium steady state, controlled by the interaction between strain-energy driven undercutting dissolution and plastic flow. Undercutting dissolution reduces the area of the contact, and preferentially removes regions with high dislocation density, while plastic flow increases the contact area by mobilizing dislocations that strain harden the crystal. The feedback between these two mechanisms drives the system towards a dynamic steady state.

8:36AM A8.00004 Controlled Irradiative Formation of Penitentes , VANCE BERGERON, Ecole Normale Superieure, Lyon, CHARLES BERGER, Ecole Normale Superieure, Paris, M. D. BETTERTON, University of Colorado — Spike-shaped structures are produced by light-driven ablation in very different contexts. Penitentes 1-4 m high are common on Andean glaciers, where their formation changes glacier dynamics and hydrology. Laser ablation can produce cones 10-100  $\mu$ m high with a variety of proposed applications in materials science. We report the first laboratory generation of centimeter-scale snow and ice penitentes. Systematically varying conditions allows identification of the essential parameters controlling the formation of ablation structures. We demonstrate that penitente initiation and coarsening requires cold temperatures, so that ablation leads to sublimation rather than melting. Once penitentes have formed, further growth of height can occur by melting. The penitentes intially appear as small structures (3 mm high) and grow by coarsening to 1-5 cm high. Our results are an important step towards understanding and controlling ablation morphologies.

8:48AM A8.00005 Transient growth and controlled side branching of xenon dendrites, MARCO FELL, J. H. BILGRAM, ETH Zurich, Switzerland — In our experiments we study the influence of transient growth conditions on the growth of xenon dendrites from undercooled melt. Here we report on the response of crystal growth on heating the melt. We start heating at a given temperature and steady-state growth. The dendrite tip reacts on this change by slowing down growth rate v and increasing tip radius R. We observe that side branches emerge from an unstable surface. As we continue heating up to slightly above melting temperature, the tip radius continuously decreases to a new value. The reverse temperature change unveils a hysteretic behavior: As soon as we cool down the melt from a temperature tight above melting temperature, v and R both increase. The curvature of the tip becomes too small to be stable at the given undercooling and an instability leads to a new, thin tip growing out of the oversized sphere-like tip. The value  $R^2v$  shows a sharp peak and then settles to a constant value in only about 20 seconds. The same instability also gives rise to side branches whose formation can be controlled by a repetitive application of the described mechanisms. Highly symmetric xenon crystals can be grown by this technique.

9:00AM A8.00006 Late time growth dynamics in the Cahn-Hilliard equation<sup>1</sup>, TMOTHY S. SULLIVAN, Department of Physics, Kenyon College, P. PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University — Numerical simulations were carried out in 2D of the scaled Cahn-Hilliard equation  $\left[\partial\psi/\partial t = (1/2)\nabla^2(-\psi+\psi^3-\nabla^2\psi)\right]$  starting from Gaussian distributed, random initial conditions on a 540x540 square grid. Simulations were run for a dimensionless time of 200,000, a factor of ten beyond previously reported results. The simulations also covered a broad range of values of the mean composition, including several at values that had not previously been reported. For each composition and for time intervals of no longer than 5000 in dimensionless time, the structure factor was calculated for sixty separate runs and averaged. The pair correlation function was then calculated from the average structure factor and its first zero crossing,  $R_G(t)$ , taken as a measure of the average domain size, was determined. An equation of the form  $R_G(t) = at^b + c$  was then fit to our data over the dimensionless time range from 5000 to 200,000. In contrast to previous work, we find that the scaling exponent *b* varies with mean composition and does not appear to be consistent with the Lifshitz-Slyozov result b = 1/3. The largest deviation occurs at a mean composition of 0.2, where  $b = 0.244 \pm 0.003$ . We discuss the possible effects of morphology on both the scaling law and the time it takes to reach the scaling regime.

<sup>1</sup>Work supported by Kenyon College, the Liquid Crystal Institute, and The Ohio Supercomputer Center

9:12AM A8.00007 Domain Growth in 2D Hexagonal Patterns with Diffuse Interfaces, DANIEL A. VEGA, LEOPOLDO R. GÓMEZ, Department of Physics - Universidad Nacional del Sur - CONICET. (8000) - Bahía Blanca - Argentina, RICARDO J. PIGNOL, Department of Mathematics - Universidad Nacional del Sur. (8000) - Bahía Blanca - Argentina — The coarsening process in planar patterns has been extensively studied during the last two decades. Although progress has been made in this area, there are still many open questions concerning the basic mechanisms leading the system towards equilibrium. Some of these mechanisms (including curvature driven growth, grain rotation and defect annihilation) have mostly been addressed in systems displaying sharp interfaces. In this work we traced the dynamics of phase separation in hexagonal patterns with diffuse interfaces through the Cahn-Hilliard model. By studying orientational and translational order and densities of topological defects we were able to identify a mechanism of coarsening simultaneously involving curvature driven growth, front propagation and grain rotation. In this regime we found that different correlation lengths characterizing the hexagonal pattern increase logarithmically with time.

9:24AM A8.00008 Oscillatory patterns near the instability threshold in extended systems with reflection symmetry, ALEXANDER NEPOMNYASHCHY, IRINA SMAGIN, Technion, Haifa, Israel, VLADIMIR VOLPERT, ALEXANDER GOLOVIN, Northwestern University — It is well known that the envelope function of a modulated traveling wave spontaneously generated by a shortwave instability is governed by a complex Ginzburg-Landau equation (CGLE). Various modulation phenomena, which include the nonlinear development of a modulational instability of periodic waves in the supercritical region, as well as the formation of stable modulated waves in the subcritical region, have been extensively studied in the framework of CGLE. The nonlinear interaction between two waves moving in the opposite directions is described by a system of two non-locally coupled CGLEs that has not been studied in detail yet. We use this system for studying several phenomena related to modulated waves. The results are applied to problems of transverse instabilities of fronts in combustion and explosive crystallization.

9:36AM A8.00009 Effects of the Deep of Quench on the Mechanisms of Pattern Formation of Sphere Forming Block Copolymers, LEOPOLDO R. GÓMEZ, DANIEL A. VEGA, Department of Physics - Universidad Nacional del Sur - CONICET. (8000) - Bahía Blanca - Argentina, ENRIQUE M. VALLÉS, Plapiqui - Universidad Nacional del Sur - CONICET. (8000) - Bahía Blanca - Argentina, ENRIQUE M. VALLÉS, Plapiqui - Universidad Nacional del Sur - CONICET. (8000) - Bahía Blanca - Argentina, ENRIQUE M. VALLÉS, Plapiqui - Universidad Nacional del Sur - CONICET. (8000) - Bahía Blanca - Argentina - The disorder-order transition of a two dimensional sphere forming block copolymer is studied through the Cahn-Hilliard model at different deeps of quench. The process of microphase separation and kinetic of pattern formation are controlled by the spinodal and order-disorder temperatures. In the spinodal region the deep of quench strongly affect both, ordering times and density of topological defects. As the spinodal temperature is approached, the density of disclination becomes very small and grains show a perfect orientational and translational order. In a narrow region of temperatures the system relax towards equilibrium via the nucleation and growth mechanism. In this region the critical grain size is approximately one lattice constant in the neighborhood of the spinodal line and diverges as the order-disorder temperature is approached.

9:48AM A8.00010 Feedback Control of Pattern Formation, LIAM STANTON, ALEXANDER GOLOVIN, Northwestern University — Global feedback control of spatially-regular patterns described by the Swift-Hohenberg (SH) equation is studied. Two cases are considered: (i) the effect of control on the competition between roll and hexagonal patterns; (ii) the suppression of sub-critical instability by feedback control. In case (i), it is shown that control can change the stability boundaries of hexagons and rolls. Particularly, for certain values of the control parameter, both hexagons and rolls are unstable, and one observes non-stationary patterns with defects. In case (ii), the feedback control suppresses the unbounded solutions of a sub-critical SH equation and leads to the formation of spatially-localized patterns.

#### 10:00AM A8.00011 Grain boundary stability in stripe configurations of non potential, pattern

forming systems, JORGE VINALS, ZHI-FENG HUANG, McGill University — We describe numerical solutions of nonpotential models of pattern formation in non equilibrium systems to address the motion of grain boundaries separating large domains of stripe configurations. One of the models allows for mean flows. Wavenumber selection at the boundaries, boundary instability, and defect formation and motion at the boundary are described as a function of the distance to onset.

10:12AM A8.00012 Mesoscale Theory of Grains and Cells: Crystal Plasticity and Coarsening<sup>1</sup>, SURACHATE LIMKUMNERD, JAMES SETHNA, Laboratory of Atomic and Solid State Physics, Cornell University — Line-like topological defects inside metals are called dislocations. At high temperatures, polycrystalline grains form from the melt and coarsen with time: these dislocations can both climb and glide. At low temperatures under shear the dislocations (which allow only glide) form into cell structures. While both the microscopic laws of dislocation motion and the macroscopic laws of coarsening and plastic deformation are well studied, we have had no simple, continuum explanation for the evolution of dislocations into sharp walls. We present here a mesoscale theory of dislocation motion which provides a quantitative description of deformation and rotation, grounded in a microscopic roder parameter field exhibiting the topologically conserved quantities. The topological current of the Nye dislocation density tensor is derived from a microscopic theory of glide driven by Peach-Koehler forces between dislocations using a simple closure approximation. The evolution law leads to singularity formation in finite time, both with and without dislocation climb. Implementation of finite difference simulations using the upwind scheme and the results in one and higher dimensions will be discussed.

 $^1\mathrm{ITR}/\mathrm{ASP}$  ACI0085969 and DMR-0218475

#### 10:24AM A8.00013 Numerical Studies of annular electroconvection in the weakly nonlinear

**regime**, PEICHUN TSAI, Department of Physics, University of Toronto, ZAHIR A. DAYA, Defence R&D Canada, STEPHEN W. MORRIS, Department of Physics, University of Toronto — We study 2D electrically-driven convection in an annular geometry by direct numerical simulation. The simulation models a real experiment which consists of a weakly conducting, submicron thick liquid crystal film suspended between two concentric electrodes. The film is driven to convect by imposing a sufficiently large voltage V across it. The flow is driven by a surface charge density inversion which is unstable to the electrical force. This instability is closely analogous to the mass density inversion which is unstable to the buoyancy force in conventional thermally-driven Rayleigh-Bénard convection. The important dimensionless parameters are a Rayleigh-like number R, proportional to  $V^2$ , a Prandtl-like number P, equal to the ratio of the charge and viscous relaxation times, and the radius ratio  $\alpha$ , characterizing the annular geometry. The simulation uses a pseudo-spectral method with Chebyshev polynomials in the radial direction and Fourier modes in the azimuthal direction. We deduce the coefficient g of the leading cubic nonlinearity in the Landau amplitude equation from the computed amplitude of convection. We investigate the dependence of g on  $\alpha$  and P and compare the results to experimental data and to linear and nonlinear theory.

10:36AM A8.00014 Demodulation of Electroconvective patterns in Nematic Liquid Crystals<sup>1</sup>, GYANU ACHARYA, Kent State University, JOSHUA LADD, Colorado State University, J.T. GLEESON, Kent State University, IULIANA OPREA, GERHARD DANGELMAYR, Colorado State University — We present the results of pattern formation in electroconvection of liquid crystal 4-ethyl-2-fluoro-4'-[2-(trans-4pentylclohexyl)-ethyl]biphenyl(J52) with planar alignment. The pattern was a function of three control parameters: applied ac voltage, driving frequency and electrical conductivity. Over certain range of conductivity, the initial transition (supercritical Hopf bifurcation) leads to right and left traveling zig and zag rolls .For the demodulation of images, Fourier transform (FT) of a time series of images were taken with the sampling rate greater than the Hopf frequency. To demodulate zig/zag rolls, the region around  $k_n$  (the wave vector of a given mode) of interest at one quarter of the FT was taken setting all FTs zero. Taking the index of the maximum FT value at that region as the reference point, again this region was separated into four parts and redistributed at four corners. The absolute value of the inverse FT of the modified function gives the required envelope.

<sup>1</sup>supported by NSF-DMS0407418

10:48AM A8.00015 Pattern Formation and Dynamics in Electroconvection of Nematic Liquid Crystals: a Theoretical and Experimental Study of the Weak Electrolyte Model<sup>1</sup>, IULIANA OPREA, Colorado State University, J.T. GLEESON, Kent State University, GERHARD DANGELMAYR, Colorado State University — Ginzburg Landau formalism is used in the study of electrohydrodynamic convection in a planar layer of nematic liquid crystal based on the weak electrolyte model. Stable wave patterns predicted by weak electrolyte model near a Hopf bifurcation of the basic state are analyzed and bounds for the Eckhaus stability are obtained. The weak electrolyte model, that treats the conductivity as a dynamical variable, is tested by quantitative comparison of experimentally measured and theoretically calculations of specific parameters, such as the recombination rate and charge transport, for the nematic I52. The experimentally observed spatiotemporal chaos evolving at the onset is qualitatively compared with the spatiotemporal chaos obtained in the numerical simulations of the four globally coupled Ginzburg Landau equations describing the dynamics of the amplitudes of the bifurcated patterns.

<sup>1</sup>Supported by NSF DMS-0407418

#### Monday, March 13, 2006 8:00AM - 11:00AM – Session A21 DFD: Colloids I: Emulsions, Foams, and Suspensions Baltimore Convention Center 318

8:00AM A21.00001 Bubble size distribution in a steady-state column of aqueous foam. , KLEBERT FEITOSA, DOUGLAS J. DURIAN, University of Pennsylvania — We report on measurements of the distribution of bubble sizes in a vertical column of aqueous foam. The sample is generated and maintained in steady-state by continuous bubbling of gas  $(CO_2)$  in a surfactant solution  $(H_2O + AOS + NaCI)$  at the bottom of a tall Lucite cylinder. The constant flow of gas produces nearly identical bubbles that accumulate at the liquid/foam interface and subsequently move up with constant velocity. The distribution of bubble sizes depends on height, being monodisperse near the bottom, turning bidisperse at some intermediate height, and then becoming polydisperse further up in the column. This behavior is exclusively due to coarsening and drainage, since film-rupture and convection are not observed. The development of a bidisperse distribution cannot be explained by mean-field theories of coarsening, in which bubbles of a given size grow or shrink at a rate that depends only on their size in comparison with a mean size.

8:12AM A21.00002 Rheology of Foams Bubble by Bubble, STEPHAN KOEHLER, Physics, Emory University — We present rheological measurements of single bubbles, and collections of bubbles to investigate cooperative effects between the bubbles that comprise a foam. For small numbers of monodisperse bubbles we measure the elastic behavior and yield stresses, and make comparisons with polydisperse foams composed of many bubbles. We also present a technique for measuring an ageless foam, where the bubble size and liquid volume fraction remain constant, outside of a microgravity environment.

8:24AM A21.00003 Pattern formation in flowing foams. , SOMA SANYAL, JAMES GLAZIER, Indiana University — We report on a new fingering morphology which an expanding air bubble generates in a foam flowing due to an applied pressure across a Hele-Shaw cell. Previous studies have only looked at patterning when the background is stationary. Our simulations using the Glazier & Grainer's Cellular Potts model show that the transition between the different morphologies depend on the rate of bubble flow into the foam. Since the rate of bubble in-flow is related to the shear strain rate, this agrees with previous experiments which have shown fingering morphologies in foams depend on the shear strain rate. The new mushroom morphology occurs for a high rate of bubble inflow corresponding to a very low shear strain rate. It is associated with a highly non-uniform velocity profile of the bubbles in the foam. These new morphologies should be easy to observe experimentally.

8:36AM A21.00004 Rigidity percolation in foamy sands, SYLVIE COHEN-ADDAD, REINHARD HOHLER, MARCEL KRZAN, MARIJO MARINIC, Universite de Marne-la-Vallee, BENJAMIN HERZHAFT, Institut Francais du Petrole — When subjected to a small shear stress, an aqueous foam behaves as a linear viscoelastic materials, whereas large applied shear stress triggers bubble rearrangement which causes the foam to flow as a viscous liquid. The elastic behavior arises from the surface tension of the gas-liquid interfaces. We study experimentally how the shear modulus and the yield stress of foam are modified if non colloidal solid particles of controlled size are dispersed in the sample. We show that even small amounts of non colloidal particles of controlled size are dispersed in the sample. We show that even small amounts of non colloidal particles of controlled size are dispersed in the sample. We show that even small amounts of non colloidal particles of controlled size are dispersed in the sample. We show that even small amounts of non colloidal particles of controlled size are dispersed in the sample. We show that even small amounts of non colloidal particles of controlled size are dispersed in the sample. We show that even small amounts of non colloidal particles of the elasticity enhancement with solid fraction qualitatively agrees with that predicted by an effective medium rigidity percolation model in the superelastic limit. To gain insight about the interactions between solid particles that are involved in the rigidity percolation, we study the dependence of the percolation threshold with particle to bubble size ratio.

#### 8:48AM A21.00005 Diffusive liquid transport in poroelastic materials : the case of foams in

**microgravity**, ARNAUD SAINT-JALMES, SEBASTIEN MARZE, HERNAN RITACCO, DOMINIQUE LANGEVIN, Laboratoire de Physique des Solides, Universite Paris-Sud, Orsay — On Earth, the liquid inside an aqueous foam irreversibly flows due to coupled gravitational and capillary effects. In microgravity, one can study liquid transport with only capillarity as a driving force. Here, we report results of capillary imbibition experiments performed in parabolic flights in which we follow how and where some liquid locally injected into a foam spreads with time. Different setup geometries, imbibition modes and bubble surface mobilities are studied. New behaviors, not observed on ground, with high liquid fractions are found. Comparisons with theoretical models are presented, allowing us to find their limits of validity as the liquid fraction is increased. These experiments also give us some insights on the convective instability occurring on ground, and allow us to discuss the analogy with diffusive liquid transport and swelling in other porcelastic materials, like plants and tissues. 9:00AM A21.00006 Structure and dynamics of foam-like emulsions , VINOTHAN MANOHARAN, Dept of Physics and Division of Engineering and Applied Sciences, Harvard University, JOHN C. CROCKER, Chemical and Biomolecular Engineering, University of Pennsylvania — We report the results of real-space, microscopic experiments on model concentrated emulsions ( $\phi > 0.65$ ) in which the continuous and dispersed phases are both index- and density-matched. Like foams, these systems coarsen and age due to diffusion of fluid from small to large droplets, but unlike foams, they are transparent and do not drain during the course of an experiment. Thus we are able to probe their internal structure and dynamics at volume fractions ranging from 0.65 to 0.90. Measurements of the mean-squared displacement of small tracer particles embedded in the emulsion reveal that the system exhibits non-thermal stress fluctuations with Lorentzian power spectral density. We relate these fluctuations to intermittent droplet rearrangements, presumably driven by coarsening, that we observe directly through confocal microscopy.

9:12AM A21.00007 Mean Field Theory of Foam Aging, OLIVIA HALT, University of Pennsylvania, RANDALL KAMIEN, University of Pennsylvania — We describe our work on the geometrical properties of a random foam as a function of the number of faces, based on Isotropic Plateau Polyhedra [1,2]. Analytic values of specific area, the stretching moment, and curvature can be obtained for these geometrical constructs. The expression for curvature is a ratio of the volume to the area of the foam cell. Focusing on this quantity will allow a better description of the coarsening of a foam. Conclusions from this mean field study will be discussed. [1] Glicksman M., *Phil. Mag.*, **85** (2005) 3. [2] Hilgenfeldt S., Kraynik A., Reinelt D., and Sullivan J. *Europhys. Lett.* **67** (2004) 484.

9:24AM A21.00008 Emulsions Droplet Capture Mechanism in Porous Media, KHALIL ZEIDANI, MARCEL POLIKAR, University of Alberta — This study was undertaken to investigate the physics of emulsion flow in porous media. The objective of experiments were to study the applicability of oil-in-water emulsion as a plugging agent in the vicinity of the well bore for thousands of Canadian gas wells that are continuously leaking gas to surface. The motion of oil droplets and the capture mechanisms were investigated through visualized experiments. Well-characterized emulsions were injected into a micro model resembling a two parallel plate model packed with glass beads. Effects of emulsion properties and wettability of the medium were studied on a plugging mechanism. The results demonstrate the reduction in permeability mainly due to droplets size exclusion compared to the pore constrictions. Also, smaller droplets may lodge and coalesce in pores crevices thereby accelerating the blockage process. Moreover, more viscous emulsions are more effective compared with the less viscous ones due to combined effects of capillary and viscous forces. The deposition of droplets was adjusted through utilizing different preflush solutions. Criteria were set for enhancing emulsion penetration depth thereby defining the extent of the blocked region. In conclusion, this work characterizes the physics of emulsion flow in porous media and demonstrates its application as a novel sealant in near well bore region. The novelty, which constitutes a step-change in technology, is a method that emplaces an emulsion at a desired location in underground media.

9:36AM A21.00009 Wigner Crystals from Charge Stabilized Water in Oil Emulsions , MIRJAM E. LEUNISSEN, ALFONS VAN BLAADEREN, University of Utrecht, ANDREW D. HOLLINGSWORTH, MATT SULLIVAN, Princeton University, PAUL CHAIKIN, New York University, SOFT CONDENSED MATTER GROUP COLLABORATION, PRINCETON INSTITUTE FOR THE SCIENCE AND TECHNOLOGY OF MATERIALS COLLABORATION — A drop of water shaken or sonicated in a CHB-Decalin oil mixture produces a stable emulsion of 1-100 micron scale water droplets. The interdroplet correlations indicate strong electrostatic repulsion. When the preparation is by sonication the particle size is smaller and more uniform and the water droplets arrange in a BCC structure characteristic of a Wigner Crystal. The lattice constants are up to 20 microns. We suggest that the water droplets deionize the organic solvent due to water's high dielectric constant and hydration energy. This decreases the electrostatic screening. A slight preference of the water hydration energy for different ionic species will lead to slightly larger droplet uptake of one charge over the other and will result in the droplets being charged. The amount of charging can be controlled by changing pH. Experiments with oil-water and colloids will also be discussed.

9:48AM A21.00010 Microrheological Study of the Time Dependent Gelation of Single Wall Carbon Nanotube Suspensions, D.T.N. CHEN, L.A. HOUGH, M.F. ISLAM, A.G. YODH, Dept. of Physics & Astronomy, University of Pennsylvania — Single wall carbon nanotubes (SWNTs) dispersed in water using an anionic surfactant, sodium dodecylbenzene sulfonate (NaDDBS) form reversible gels because of the bonding between the individual nanotubes (L.A. Hough, M.F. Islam, P.A. Janmey and A. G. Yodh Phys. Rev. Lett. 93, 168102 (2004)). We study the time dependence of this reversible gelation using particle tracking microrheology. We empirically collapse the mean square displacement onto a single master curve that extends over several decades in time using a time-cure superposition. The frequency scaling exhibited by the viscoelastic moduli obtained from the master curve is remarkably similar to that of semiflexible polymer networks. By comparing the results from a range of initial SWNT supported by the NSF through Grants DMR 05-20020 (MRSEC) and DMR-0505048, and by NASA grant NAG8-2172.

10:00AM A21.00011 Yielding and flow of soft particle dispersions: the role of elastohydrodynamic interactions. , MICHEL CLOITRE, Matiere Molle et Chimie (UMR ESPCI-CNRS 7167), ESPCI, 10 rue Vauquelin, Paris, France, JYOTI SETH, ROGER BONNECAZE, Department of Chemical Engineering and Texas Materials Institute, The University of Texas at Austin, Austin, Texas 78172, USA — Concentrated dispersions of soft particles such as emulsions, colloidal pastes and granular suspensions exhibit many fascinating phenomena such as yielding, shear thinning, aging and memory, slip and fracture. Elucidating the physical parameters controlling these properties and the mechanisms at work is a formidable challenge. Recently we have found that various soft particle pastes share in common universal flow properties that can be characterized with very simple constitutive equations involving the solvent viscosity, the bulk elasticity and geometrical factors. We shall describe a generic flow model based on internal slip and non-contact elasto-hydrodynamic forces between squeezed particles<sup>1</sup> that quantitatively accounts for the measured properties. This approach offers new routes to predict the bulk non-linear rheology of pastes. <sup>1</sup>S.P. Meeker, R.T. Bonnecaze, M. Cloitre, *Phys. Rev. Lett.* **92**, n° 198302 (2004).

10:12AM A21.00012 Mixture Stress in a Non-Uniform Suspension<sup>1</sup>, QUAN ZHANG, ANDREA PROSPERETTI<sup>2</sup>, Johns Hopkins University — In nature, most suspensions are non-uniform and the particles are subjected to external forces, such as gravity. The external force induces relative motions between the particles and the fluid, which introduce a new degree of freedom. We investigate the ensemble averaged stress system in a non-uniform suspension of equal spheres with external forces. It is found that, as a consequence of the spatial non-uniformity of the particle distribution and the relative motion between the two phases, new terms arise in the symmetric part of the bulk stress. In addition, an anti-symmetric contribution is found even in the absence of external torques. All the new terms in the stress tensor depend on the particle volume fraction and the gradient of the relative velocity but, for a given volume fraction, are independent of the particle size. To determine the new transport coefficients for small volume fractions, the renormalization, from which the new transport coefficients are calculated. The numerical results agree well with the dilute limit calculations.

<sup>1</sup>Supported by NASA and NSF <sup>2</sup>University of Twente and Burgerscentrum 10:24AM A21.00013 Brownian Motion of an ellipsoid<sup>1</sup>, YILONG HAN, Department of Physics and Astronomy; University of Pennsylvania, AHMED ALSAYED, MAURIZIO NOBILI, CNRS-University Montpellier II, France, JIAN ZHANG, TOM LUBENSKY, ARJUN YODH — We report direct digital-video-microscopy measurements of the Brownian motion of isolated anisotropic (ellipsoidal) particles in water under quasi-2D confinement. The probability density function (PDF) of displacements in the lab-frame is found to be nonGaussian. This effect originates from the anisotropy of the hydrodynamic drag coefficient. The transition from anisotropic to isotropic diffusion and the correlations between translational and rotational motions are also measured. The observations are confirmed numerically and understood theoretically via a Langevin formalism. We also observed the ratio of diffusion coefficients,  $D_a/D_b$ , along long and short axes, respectively, could be larger than 2, the theoretical upper limit in three dimension.

#### <sup>1</sup>ACKNOWLEDGE GRANTS: DMR05-20020

10:36AM A21.00014 Sound propagation in nanofluids , X. XIE, R. ANNAMALAI, R. SOORYAKUMAR, D. STROUD, V. SUBRAMANIAM, J. HEREMANS, The Ohio State University — The thermal properties of nanofluids, i.e. liquids containing nanoparticles of sizes in the 3 to 100 nm range, have recently been shown to exhibit an unexpectedly large enhancement in thermal conductivity. While this enhancement has been observed for metallic nanoparticles and carbon nanotubes, the physical origin of the enhancement remains to be understood. The propagation of acoustic waves through a nanoparticle-laden colloidal fluid system offers many advantages towards understanding its thermal properties. We report on results of Brillouin scattering which probes the frequency range of  $\sim 1 - 100$  GHz to study sound propagation in such complex fluids which possess structures on length scales larger than the molecules that comprise the host fluid. Thus compared to simple liquids, nanofluids possess additional relaxation mechanisms that can be observed in the frequency dispersion of the sound propagation. We present light scattering results from nanofluids comprised of a suspension of relatively long  $(1 - 2 \mu m) 20$  nm diameter single-walled carbon nanotube bundles dispersed in N,N dimethylformamide.

10:48AM A21.00015 Electrokinetic Phenomena of Colloidal Suspensions , JIAN LIU, Department of Physics and Texas Center for Superconductivity, University of Houston, 202 Houston Science Center, Houston, Texas 77204-5002, JASON SHULMAN, Department of Physics and Texas Center for Superconductivity, University of Houston, 202 Houston Science Center, Houston, Texas 77204-5002, YUYI XUE, Department of Physics and Texas Center for Superconductivity, University of Houston, 202 Houston Science Center, Houston, Texas 77204-5002, FENG CHEN, Department of Physics and Texas Center for Superconductivity, University of Houston, 202 Houston Science Center, Houston, Texas 77204-5002, CHING-WU CHU<sup>\*</sup>, Department of Physics and Texas Center for Superconductivity, University of Houston, 202 Houston Science Center, Houston, Texas 77204-5002, CHING-WU CHU<sup>\*</sup>, Department of Physics and Texas Center for Superconductivity, University of Houston, 202 Houston Science Center, Houston, Texas 77204-5002, CHING-WU CHU<sup>\*</sup>, Department of Physics and Texas Center for Superconductivity, University of Houston, 202 Houston Science Center, Houston, Texas 77204-5002, CHING-WU CHU<sup>\*</sup>, Department of Physics and Texas Center for Superconductivity, University of Houston, 202 Houston Science Center, Houston, Texas 77204-5002 — We investigate the colloidal particle motion of colloid suspension in which giant electrorheological effect has been found. The colloids consist of urea coated  $Ba_{0.8}Rb_{0.4}TiO(C_2O_4)_2$  particles suspended in silicon oil. In the experiment, a cell with cross-aligned top and bottom stripe-electrodes is used. The electric potential, the field and the field gradient, therefore, possess different space distribution. Significant difference of colloids motions and equilibrium particle distributions are observed under ac, dc and ac+dc fields. The result suggests dipole may not be the only factor for colloid aggregation (meso-structure), and hence, its electrorheological effect. \*also at Hong Kong University of Science and Technolog

#### Monday, March 13, 2006 11:15AM - 2:15PM – Session B8 GSNP DFD: Focus Session: Granular Materials Near Jamming Baltimore Convention Center 314

11:15AM B8.00001 Elastic Granular Flows , CHARLES CAMPBELL, University of Southern California — There is no fundamental understanding of the mechanics of granular solids. Partially this is because granular flows have historically been divided into two very distinct flow regimes, (1) the slow, quasistatic regime, in which the bulk friction coefficient is taken to be a material constant, and (2) the fast, rapid-flow regime, where the particles interact collisionally. But slow hopper flow simulations indicate that the bulk friction coefficient is not a constant. Rapidly moving large scale landslide simulations never entered the collisional regime and operate in a separate intermediate flow regime. In other words, most realistic granular flows are not described by either the quasistatic or rapid flow models and it is high time that the field look beyond those early models. This talk will discuss computer simulation studies that draw out the entire flowmap of shearing granular materials, spanning the quasistatic, rapid and the intermediate regimes. The key was to include the elastic properties were previously unnecessary in the plasticity and kinetic theory formalisms that respectively form the foundations of the quasistatic and rapid-flow theories. Granular flows can now be divided into two broad categories, the Elastic Regimes, in which the particles are locked in force chains. The Elastic regimes can be further subdivided into the Elastic-Quasistatic regime (the old quasistatic regime) and the Elastic-Inertial regime. The Elastic-Inertial regime is the "new" regime conserved in the landslide simulations, in which the inertially induced stresses are significant compared to the elastically induced stresses. The lenetial regime is a range of dense concentrations ( $0.5 < \nu < 0.6$ ) in which it is possible, but not necessary to form force chains and demonstrate elastic behavior. (In other words it is possible for the material to exhibit two different states at the same concentration.) By forcing the material to suppor

#### 11:51AM B8.00002 Force distributions and stress fluctuations in a triangular lattice of rigid

**bars**<sup>1</sup>, BRIAN TIGHE, JOSHUA SOCOLAR, Physics Dept., Duke University, Durham, NC — We study the uniformly weighted ensemble of force balanced configurations on a triangular network of nontensile contact forces as a model of force distribution on a hyperstatic granular material. For periodic boundary conditions corresponding to isotropic compressive stress, the probability distribution for single-contact forces, P(f), decays faster than exponentially, and a field closely related to the lattice version of the Airy stress function is found to have fluctuations characterized by a structure factor  $S(q) \sim 1/q^4$ . The super-exponential decay of P(f) persists in lattices diluted to the rigidity percolation threshold. On the other hand, for anisotropic imposed stresses, a broader tail emerges, becoming a pure exponential in the limit of infinite lattice size and infinitely strong anisotropy.

<sup>1</sup>Supported by NSF Grants No. DMR-0137119 and DMS-0244492.

#### 12:03PM B8.00003 Measurement of Forces inside Three-Dimensional, Frictionless, Disordered

Matter, JING ZHOU, ANTHONY DINSMORE, University of Massachusetts at Amherst — We directly measured individual forces inside the concentrated piles of frictionless droplets. We report on the distribution of contact forces normalized by the droplet mean, in addition to the distribution of forces normalized by sample mean, as well as the distribution of contact angles. We compare these results to existing models and to a new, numerical calculation that treats the droplets as independent particles and derive the contact-force probability distribution that arises self-consistently from balancing forces. The force chain architecture was visualized, and quantified with a new definition based on long-range correlations. The obtained chain persistence length helps to establish a connection between microscopic force network and the modulus of meso- or macroscopic piles. This work is supported by NSF (DMR-0305395).

12:15PM B8.00004 Effects of Particle Size Dispersity on the Response to Compressive Strains<sup>1</sup>, MEENAKSHI DUTT, University of Cambridge, BRUNO HANCOCK, Pfizer Inc., Groton, Connecticut, USA, CRAIG BENTHAM, Pfizer Ltd., Sandwich, Kent, USA, JAMES ELLIOTT, University of Cambridge — Particle packings found in nature and industry are rarely comprised of single components, in terms of particle size. These packings are generated under a variety of circumstances which influence its response to an external load or strain. We explore both the effect of packing history prior to application of compressive strain, and the variation in the response with the size distribution of the component particles. We generate the packings by allowing the particles to settle under gravity for a fixed interval of time, or until a cut-off packing fraction is attained, followed by application of a compressive strain for a fixed interval of time. We repeat these studies using numerical experiments for samples of discrete size (200 microns, 195-225 microns, 170-260 microns, 150-295 microns) and random (100-300 microns, 100-400 microns, 100-500 microns) size distributions. We find the number of particles with fewer than 4 contacts to increase with size dispersity of the sample after the particles settle under gravity. In addition, the fraction of plastic contacts decreases with increasing variation in particle size during the compression. We also present correlations between the populations of low and high force bearing contacts, particle size and the yield state of the contacts.

<sup>1</sup>Special Acknowledgements to Pfizer for funding

12:27PM B8.00005 Measurements of the Yield Stress in Repulsive Athermal Systems , NING XU, COREY O'HERN, Yale University — We performed molecular dynamics of dry frictionless granular media to gain a deeper understanding of the yield shear stress in these materials. The measurements were obtained by shearing the systems in both the constant shear force and constant shear velocity ensembles. At fixed shear force, we identified the yield shear stress as the shear stress  $\Sigma_{yf}$  required to maintain steady flow in an initially unsheared static state. At fixed shear velocity, we identified the yield shear stress as the average shear stress  $\Sigma_{yv}$  in the limit of zero shear velocity. At finite system size,  $\Sigma_{yf} > \Sigma_{yv}$ , which implies that there is a shear rate discontinuity when the system begins flowing in the constant shear force ensemble. However, the difference between the two measures of the yield shear stress with increasing system size;  $\Sigma_{yf}$  and  $\Sigma_{yv}$  become identical in the infinite system size limit. Thus, the jump discontinuity in the shear rate at the unjamming threshold is a finite-size effect in frictionless granular systems.

12:39PM B8.00006 Experiment test of a Janssen formula in a dense granular column<sup>1</sup>, KEVIN FACTO, University of Massachusetts-Amherst, TOM SCHICKER, University of Massachusetts-Amherst, NARAYANAN MENON, University of Massachusetts-Amherst — The stresses inside a tall column of either static or flowing granular material saturate with depth, because the weight of the material is borne by friction with the walls. In the static case, the height dependence of the stress is traditionally described by the Janssen formulation, in which the shear stress at the wall is assumed to be proportional to the normal stress. We report measurements of all three components of force at the wall of a dense, gravity-driven flow of glass beads. We find that the depth dependence of the stress in this slow flow is well-described by a Janssen-like formula. We are also able for the first time to directly test the Janssen assumption, and find that the fluctuations in the shear and normal forces at the wall are highly correlated. The measured friction angle is independent of flow rates for the slow flows we have examined, and is surprisingly close to the ensemble average of the friction angle measured when the flow is stopped.

 $^1\mathrm{We}$  acknowledge support from NSF-DMR 0303596

12:51PM B8.00007 Impact of Particle Elasticity on Granular Force Networks , JOHN WAMBAUGH, Duke University, ANNIE THEBPRASITH, Mount Holyoke College, ROBERT HARTLEY, Duke University, ROBERT BEHRINGER, Duke University — We investigate the distribution of force within vertically-confined granular assemblies using photoelastic techniques that allow determination of both geometric configuration and force upon each particle. By binning multiple realizations with depth, we are able to compare our results with the simple, continuum model of Janssen. Recent experimental studies of the force at the boundaries of such assemblies have largely confirmed Janssen's prediction that mean force saturates exponentially with depth due to frictional contacts at the boundaries. [Ovarlez, Fond and Clement, PRE 67, 060302 (2003)] We have observed deviations from these predictions in our system, which we quantify in terms of the structure of the network that distributes forces. We examine the role of internal elasticity of the particles in causing these deviations. This research is supported by NSF grants DMR-0137119 and DMS-204677 and NASA grant NNC04GB08G.

1:03PM B8.00008 Freezing and Melting in Granular Materials , KAREN DANIELS, Dept. of Physics, North Carolina State University — From bowls of nuts to eroding soil, granular materials are all around us. In spite of the fact that granular materials are dissipative and athermal, statistical mechanics allows considerable insight into their behavior. I will present experiments on particles which are vibrated from below and sheared from above within an annular channel. The vibrations have the remarkable effect of crystallizing the material, rather than melting it as temperature would an ordinary material. This freezing/melting transition is hysteretic, with the critical line corresponding to equal kinetic energies for vibration and shear. We characterize the transition between these two states, and observe features reminiscent of both a jamming transition and critical phenomena. Another remarkable property is the increase of pressure with volume over a continuum of partially and/or intermittently melted states, in contrast to standard thermodynamic behavior.

1:39PM B8.00009 Plastic Failure Events in 2D Sheared Granular Systems<sup>1</sup>, TRUSH MAJMUDAR, ROBERT BEHRINGER, Physics Department, Duke University — We present experimental measurements of plastic failure events in a two dimensional granular system consisting of polymer photoelastic disks, placed horizontally, and confined within a rectangular biaxial cell. The bi-refringence of these disks allows us to determine the normal and tangential components of contact forces. We image the system at various deformation states and measure the stress changes and displacements of the disks during one complete shear cycle. The stress changes are found by computing the stress tensor of each disk and the displacements are measured by particle tracking. We obtain bulk stress-strain curves by spatial averaging and find that the system exhibits regions of reversible deformation interrupted by irreversible plastic failure events. We also obtain the behavior of shear modulus of the system. The spatial distribution of reversible and plastic deformations found by studying the displacements of the disks show that in two corners, the disks move uniformly but in a central band aligned along a principal strain direction, we observe multiple vortices. Reversing the direction of shear causes maximum plastic deformation which results in disruption of the vortex structure. We compare our results to the shear transformation zone (STZ) theory.

<sup>1</sup>Funding: NSF DMR - 0137119, NSF DMS - 204677, NASA - NNC04GB08G

#### 1:51PM B8.00010 Statistical Properties of Granular Solid to Liquid Transition in Small Sys-

tems under Shear, MARTIN MELHUS, IGOR ARANSON, Argonne National Laboratory, DMITRY VOLFSON, LEV TSIMRING, University of California, San Diego — The fluidization transition of a dense granular assembly under shear is studied numerically using soft particle molecular dynamics simulations in two dimensions using a previously verified predictor-corrector algorithm. We focus on small systems in a thin Couette cell, examining the bistable region while increasing shear, with varied amounts of random noise, and determine the statistics of shear required for fluidization. We find an approximately linearbetween noise and fluidization shear threshold over the transition regime, and that the variance in the threshold decreases as the system size increases.

2:03PM B8.00011 Granular shear flow with imposed vibrations, BRIAN UTTER, James Madison University, ERIC HOPPMANN, James Madison University — We present results on a 2D photoelastic shearing experiment in which we impose force fluctuations by vibrating the shearing surface. The experiment consists of a dense assembly of 2D photoelastic grains between two belts moving in opposite directions, such that the central region approximates planar shear. The granular medium lies horizontally between the belts such that gravity does not compact the grains. One of the shearing surfaces is vibrated at a known frequency and amplitude during shear. We measure properties of the particle flow and characterize the force network by placing the photoelastic grains between crossed polarizers. We find that as vibration amplitude is increased, the number and magnitude of these force chains decreases drastically. The vibration also leads to increased slip at the shearing surface and decreased particle flow at both shearing surfaces.

#### Monday, March 13, 2006 11:15AM - 2:03PM – Session B21 DFD: Colloids II: Colloidal Crystals, Gels, and Glasses Baltimore Convention Center 318

11:15AM B21.00001 Phase diagram and direct mechanical measurements of colloidal gels, NA WANG, MARIA KILFOIL — We study the phase diagram of colloidal aggregates according to different salt concentration and particle volume fraction, in the absence of gravity. This phase diagram then helps us to locate the region to form strong colloidal gels, whose mechanical properties are studied with time-sharing optical tweezers.

11:27AM B21.00002 Real Time Observations of Decaying Colloidal Clusters , MARCO POLIN, SANG-HYUK LEE, Department of Physics and Center for Soft Matter Research, New York University, WILLEM KEGEL, van 't Hoff Laboratories for Physical and Colloid Chemistry, Debye Research Institute Utrecht University, ANDREW HOLLINGSWORTH, DAVID GRIER, Department of Physics and Center for Soft Matter Research, New York University — We have studied model colloidal dispersions characterized by long-range electrostatic repulsions and short-range entropically driven attractions. Through a combination of holographic optical trapping and precision digital video microscopy we can create nonequilibrium cluster configurations and track their decay fluctuations. These measurements reveal density and shape fluctuations that accompany the decay of the clusters. Such processes may cast additional light on decay of large atomic nuclei.

11:39AM B21.00003 Length scale dependent relaxation in colloidal gels , EMANUELA DEL GADO, Dipartimento di Scienze Fisiche, Universita' degli Studi di Napoli "Federico II", WALTER KOB, Laboratoire des Cooloides, Verres et Nanomateriaux, Universite Montpellier II — Although gels are ubiquitous in fundamental science, technological applications and also in our daily life, their structural and dynamical properties are not well understood. In contrast to other systems that show a slow relaxation, such as glass-forming liquids, the structure of gels is given by an open network that is thought to be responsible for the unusual dynamical properties of these systems. We present the results of a recent study based on a simple model that does indeed have the characteristics of (colloidal) gel-forming systems at a finite temperature. By means of molecular dynamics computer simulations, we investigate the gel formation from the equilibrium sol phase. In particular we show that the strong length scale dependence of the dynamics in gel forming systems is tightly related to the formation of the gel structure and is therefore a general feature. This study allows for the first time to investigate on a microscopic level the relaxation processes in the incipient gel and to understand why they must strongly depend on the length scale investigated. In our model the mesh-size of the incipient gel network corresponds to a crossover length between dramatically different relaxation processes, from stretched to compressed exponentials. Moreover our results link the super-exponential relaxation at low temperature to the motion of pieces of the incipient gel structure.

#### 11:51AM B21.00004 Crossover from Intermittent to Continuum Dynamics for Locally Driven

**Colloids**, CHARLES REICHHARDT, CYNTHIA J. OLSON REICHHARDT, Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory — We simulate a colloid with charge  $q_d$  driven through a disordered assembly of interacting colloids with charge q and show that, for  $q_d \approx q$ , the velocity-force relation is nonlinear and the velocity fluctuations of the driven particle are highly intermittent with a 1/f characteristic. When  $q_d \gg q$ , the average velocity drops, the velocity force relation becomes linear, and the velocity fluctuations are Gaussian. We discuss the results in terms of a crossover from strongly intermittent heterogeneous dynamics to continuum dynamics. We also make several predictions for the transient response in the different regimes.

12:03PM B21.00005 Evolving Bulk Properties of Collapsing Colloidal Gels, STEPHEN KAMP, MARIA KILFOIL, McGill University — We present a study of the time evolution of the elastic properties of colloidal depletion gels. Silica colloids were suspended in NaCMC solutions and homogenized. Both the colloid volume fraction and the interaction strength (polymer concentration) were varied. The time evolution of the elastic properties of the suspensions was studied with a bulk rheometer in a double-wall Couette cell throughout the gel lifetime. The early lifetime is characterized by an elastic shear modulus that increases logarithmically with time, following which the gels experience catastrophic failure and the elastic modulus drops dramatically. As the gel collapses, various complex behaviors are seen, including a temporary stabilization against collapse, and reformation of a new gel with its own elastic properties which then follows its own trajectory to collapse. Time-lapsed images were taken of identical samples in a separate transparent cell of identical dimensions and the gel height was used to calibrate the measured shear modulus values. The visual cell also allows us to see the sample-spanning collective rearrangement involved in the collapse.

12:15PM B21.00006 Experimental characterization of the interface of a colloidal suspension. , JESSICA HERNANDEZ-GUZMAN, ERIC R. WEEKS — We investigate experimentally the interface between liquids and solids by using a suspension of colloids as our model. Their size and slow motion makes colloidal suspensions experimentally accessible using 3D high speed confocal microscopy. We track the position of the particles over time, and characterize the spatial structure using bond order parameters as has been done by previous workers. We additionally measure the mobility of each particle. We study the thickness of the interface both in terms of the static structure (which changes from liquid-like disorder to crystal-like order across the interface) and the mobility of the particles with respect to distance from the interface. We find a transition region with a thickness of a few particle diameters.

#### 12:27PM B21.00007 Freezing and Melting of Colloidal Crystals with Short-Range Attractive

**Potential**, J.R. SAVAGE, D.W. BLAIR, R.A. GUYER, A.D. DINSMORE — We study the kinetics of melting and freezing of colloidal crystals formed by a short-range attractive potential. We use aqueous suspensions of micron-sized latex spheres mixed with surfactant micelles, which create a depletion attraction among the spheres. Single- and multi-layer crystals appear on the glass surface. Upon uniformly heating or cooling, the micelles grow or shrink. Upon heating, the depletion attraction weakens by up to 0.7 kT, and the crystals melt. Optical microscopy is used to track the motions of hundreds of colloidal spheres for up to 8 hours, until crystals have melted. We initially observe a steady decrease in the size of the crystallites. When the size reaches approximately 20-30, however, crystallites rapidly shrink. Once the crystals have melted, we then supercool them and monitor the nucleation and growth of crystallites. The kinetics of individual bond-breaking events and the evolution of the crystalline order parameter in both melting and freezing will be presented. This work is supported by the NSF-DMR 0305395.

12:39PM B21.00008 Melting of Temperature-Sensitive 3D Colloidal Crystals , AHMED ALSAYED, YILONG HAN, ARJUN YODH, University of Pennsylvania — We employ thermally responsive monodisperse microgel colloidal spheres to study the melting mechanisms of colloidal crystals [1]. The particle diameter decreases with increasing temperature and leads to volume fraction changes that drive phase-transitions. We will describe observations of a variety of phenomena. Premelting, the localized loss of crystalline order near defects (e.g. grain boundaries) at volume fractions above the bulk melting transition, is directly observed by video microscopy, and is characterized by monitoring the first peak position of the particle pair correlation function. We find the position of the first peak shifts toward smaller particle separations at the onset of premelting. After Delaunay triangulation, mean square rotational and translational fluctuations of bonds were measured close to and away from defects. The behavior of all such quantities exhibits increased disorder near the defects. By locally heating the material within a crystal domain, we also studied the superheating and melting of a perfect 3D crystal. Finally, the introduction of weak attractions between spheres reveals free-floating 3D crystal 'blobs' which can be made to melt and recrystallize by tuning the temperature. [1] A. M. Alsayed, M. F. Islam, J. Zhang, P. J. Collings, A. G. Yodh, Science **309**, 1207 (2005). This work was supported by grants from NSF (DMR-0505048 and MRSEC DMR05-20020) and NASA (NAG8-2172).

# 12:51PM B21.00009 Evolution of Particle-Scale Dynamics in Suspensions of Weakly Attractive Colloids Undergoing Structural Arrest, H. GUO, D. LIANG, Johns Hopkins U., S. RAMAKRISHNAN, C.F. ZUKOSKI, UIUC, J.L. HARDEN, U. of Ottawa, R.L. LEHENY, Johns Hopkins U. — Suspensions of colloids with weak, short-range attractions can undergo an ergodic to nonergodic transition (ENT) as the strength of the attraction or the particle concentration increases. At low densities the transition corresponds to gelation, while at high densities it is identified as an attractive glass transition. We employ x-ray photon correlation spectroscopy (XPCS) to investigate the slowing dynamics associated the ENT in suspensions of nanometer-scale silica colloids coated with octadecyl-hydrocarbon-chains at wavevectors corresponding to interparticle length scales. At high temperatures the chains form a solvated brush that stabilizes the colloids. At low temperature, the brush collapses leading to a short-range attraction between colloids. Following a quench in temperature, the intermediate scattering function displays two features, a plateau value and a terminal relaxation time, that increase with time since the quench. A comparison between suspensions with concentrations of $\phi = 0.20$ and 0.43 shows qualitative differences in their temporal evolution, indicating a crossover from gelation-like to glass- like dynamical arrest. Further, a comparison with rheometry indicates how the slowing particle-scale dynamics correlates with the growth of the system's elastic modulus.

#### 1:03PM B21.00010 Microstructure and micromechanics of hard spheres with short-range at-

traction, MYUNG HAN LEE, ERIC M. FURST, University of Delaware — We study the microscopic mechanical response of colloidal gels, such as yielding, compression and rearrangement, by manipulating single probe particles within the network. For this work, we use fluorescent polymethylmethacrylate (PMMA) dispersed in mixtures of decalin and cyclohexylbromide, with a refractive index and density close to that of PMMA. The strength of attraction is controlled by the concentration of a non-adsorbing polymer, polystyrene, which induces a depletion attraction between particles. In the presence of sufficiently strong attractive forces, particles form a colloidal gel. Confocal microscopy is used to observe the structural evolution in real time. This enables us to investigate the role of the local structure and particle interactions in the elasticity of the network. Specifically, we identify local elastic and plastic deformations in gels, which depend on the probe oscillation amplitude and strength of attractive interactions.

1:15PM B21.00011 Deformation of Colloidal Glasses , PETER SCHALL, WZI, University of Amsterdam, ITAI COHEN, Physics Department, Cornell University, FRANS SPAEPEN, DAVID WEITZ, DEAS, Harvard University — Amorphous colloidal suspensions are known to be powerful models for studying dynamical processes in glasses. Since the particles can be observed optically in real time, colloidal systems offer the unique opportunity of studying important mechanisms at the single particle level. We use confocal microscopy to investigate structural rearrangements in colloidal glasses under applied shear. Our setup allows us to track the motion of the individual particles in three dimensions while the suspension is sheared. We use the particle positions determined by confocal microscopy to calculate the local strain tensor and to identify regions of non-affine deformation. We observe "shear zones," that are accompanied by a complex strain field around them. Using the single particle data, we elucidate the particle rearrangements in the shear zones, and we investigate correlations between the location of these shear events and regions of high free volume.

#### 1:27PM B21.00012 Rotational perturbations of colloidal suspensions near the colloidal glass

**transition.**, PIOTR HABDAS, Dept. of Physics, Saint Joseph's University, ERIC R. WEEKS, Dept. of Physics, Emory University — By increasing the concentration of small solid particles in a liquid (colloidal suspension) a colloidal glass transition is approached. This is due to the fact that the system becomes increasingly crowded and when it reaches the glass transition it becomes essentially jammed. Therefore, a colloidal suspension is a model system that exhibits a glass transition. There are a few ways of locally perturbing a colloidal suspension. For example, one of the colloidal particles can be dragged through the colloidal suspension or a dimer made out of two small particles can be rotated. To perform the latter, we mix a small number of paramagnetic beads which dense PMMA particles. Some of the beads form dimers which can be put into rotation by rotating an external permanent magnet. Using confocal microscopy we study response of the system to such local perturbation. In particular, we investigate average spatial range of these perturbations and how it varies with the rotational rate and sample concentration.

1:39PM B21.00013 Microscopy studies of the re-entrant glass transition. , ANDRZEJ LATKA, NORA GRANETO, PIOTR HABDAS, Dept. of Physics, Saint Joseph's University — Colloidal suspensions are a model system for studying the glass transition. At the volume fraction  $\phi_g \approx 0.58$  a glass transition occurs and a hard sphere colloidal glass is formed. The formation of hard sphere glass is attributed to the "caging" effect, in which the particles form cages around each other that restrict their movement. Introducing an attractive depletion force between the particles surprisingly causes the hard sphere glass to melt and the system becomes a liquid. Interestingly, by further increasing the attractive force an attractive glass is formed. Our system is a suspension of nearly hard-sphere colloidal particles and nonadsorbing linear polymer which induces a depletion attraction between the attractive glass phase.

1:51PM B21.00014 Scaling of non-linear viscoelastic transitions in soft colloidal glasses, MATTHEW HELGESON, NORMAN WAGNER, Center for Mol. and Eng. Thermodynamics, Dept. of Chemical Engineering, Univ. of Delaware, Newark, DE 19711, DIMITRIS VLASSOPOULOS, FORTH, Inst. of Electronic Structure and Laser, Gr-71110, Heraklion, Crete, Greece — Soft colloidal particles undergo a transition to a glass-like state at sufficient concentration, due to kinetic trapping, similar to the glass transition in hard sphere systems. In this work we explore the use of rheological measurements as a tool to probe the mechanisms that lead to structure formation and breakage under shear in the glassy state for a monodisperse solution of multi-arm star polymers in an athermal solvent. Maxima in the loss moduli are observed with increasing strain amplitude at the onset of shear melting. We show that the transition to non-linear viscoelastic behavior and the onset of flow follow a systematic, rate-dependent trend. Specifically the critical strain increases with frequency. We discuss this trend in terms of phenomenological understanding of the kinetic trapping of soft colloids in the glassy state, leading to characterization of the softness of the colloidal glass as well as mechanisms of shear melting.

## Monday, March 13, 2006 2:30PM - 5:30PM - Session D8 DFD GSNP: Patterns and Instabilities I Baltimore Convention Center 314

2:30PM D8.00001 Nonlinear Analysis of the Self-assembly of Nanostructures , SHAOWEN HU, University of Houston, GIRISH NATHAN, GEMUNU GUNARATNE, DONALD KOURI — We investigate properties of a model of nanoscale pattern formation on a uniform substrate. The coefficients of the Ginzburg-Landau equations are concentration dependent. We find that, above the threshold, there are two branches of solutions corresponding to the up and down hexagonal structures; their appearance is related to the initial concentration of the system. The stability of such structures is confirmed by the analysis of the phase dynamics. When system is away from the threshold, the theory predicts a competition of stripe and hexagonal structures. The predicted stability domain of the structure is is consistent with numerical simulations. This provides a framework to understand the guided self-assembly technology, e.g., by the photolithography, at a coarse scale. The possible interaction of a large scale mode with the pattern mode is also discussed.

2:42PM D8.00002 Shear band instability in the presence of convection<sup>1</sup>, SEBASTIEN AUMAITRE, J.P. GOLLUB, Haverford College — One of the main features of the atmospheric motion of giant gas planets, like Jupiter and Saturn, is their remarkably stable shear band structure. The stability and internal structure of this flow, and the consequences for the internal heat transport, are not fully understood. Here we present a flexible device to study in a laboratory experiment the stability of a shear band flow in the presence of convective heat transport. The shear band flow is generated in layer of conductive fluid by spatially periodic Lorentz forces resulting from an electric current passing through the fluid in the presence of a network of magnets placed under the cell. Moreover, a convective flow is created by an imposed temperature gradient across the fluid layer. By changing the current through the fluid, and the temperature difference across the layer, we are able to adjust independently the velocity fields resulting from the shear and thermal forcing. Heat transport, flow patterns, and velocity fields are monitored. Initial results on the threshold for the instability of the shear band flow, and the resulting flow patterns, will be presented.

<sup>1</sup>Supported by NSF-DMR -0405187.

2:54PM D8.00003 Surfactant-enhanced thermocapillary flow in two-dimensional slots. , RAM HANUMANTHU, KATHLEEN STEBE, Department of Chemical & Biomolecular Engineering; Johns Hopkins University; Baltimore, MD 21218 — An insoluble surfactant at an aqueous-gas interface can assume a variety of surface states including gaseous (G), liquid expanded (LE), and liquid condensed (LC) states. The surface pressure-surface area isotherm for such monolayers is well established; however, their thermocapillary behavior has received less attention. Recently, Nguyen & Stebe reported surfactant-enhanced Marangoni-Benard flows in evaporating aqueous drops, created by the strong dependence of surface tension on temperature in LE-LC co-existence. In this work, flow in a two-dimensional slot in the presence of insoluble surfactant is modeled. The time-dependent, incompressible Navier-Stokes equations, coupled with energy conservation and surface convection-diffusion equations are solved using Galerkin's method of weighted residuals on a finite element mesh. The model is verified against the results of Sen & Davis for steady thermocapillary flows in two-dimensional slots; and of Homsy & Meiburg for surfactant effects in a linear limit. Finally, both steady-state and dynamic flow patterns are presented that evolve when a constitutive equation that captures the full, non-linear, concentration- and temperature-dependent phase-change behavior is used. Predicted flow patterns are compared qualitatively to the experimental observations.

**3:06PM D8.00004 Weakly nonlinear dynamics of the longwave Marangoni instability in a binary-mixture layer in the presence of the Soret effect.**<sup>1</sup>, ALEXANDER ORON, Mechanical Engineering, ALLA PODOLNY, Mathematics, ALEXANDER A. NEPOMNYASHCHY, Mathematics, TECHNION-ISRAEL INSTITUTE OF TECHNOLOGY TEAM — We consider a system consisting of a layer of an incompressible binary liquid with a deformable free surface. We investigate the long-wave Marangoni instability in the case of small Lewis and Galileo numbers for finite capillary and Biot numbers in the case of a specified heat flux at the solid substrate. The Soret effect is taken into account. Both long-wave monotonic and oscillatory modes of instability are found in various parameter domains of the Biot and Soret numbers. We have derived a set of strongly nonlinear evolution equations describing the spatio-temporal dynamics of the layer in three dimensions in the case of the oscillatory instability. The weakly nonlinear analysis based on these equations demonstrates the presence of several kinds of stable supercritical standing and traveiling waves.

<sup>1</sup>The research is partially supported by the Israel Science Foundation, Grant 31/03-15.3

**3:18PM D8.00005 Convection onset in a supercritical pure fluid**, HORST MEYER, Duke University — The convection onset of a pure supercritical fluid  ${}^{-3}$ He - in a Rayleigh-Bénard cell has been investigated along the critical isochore by measuring the temperature drop  $\Delta T(t)$  across the fluid layer as a function of time t after starting the heat current q. The measurements showed after the initial sharp rise in  $\Delta T(t)$  a first maximum at the time  $t_p$ , which indicates that the convection has developed and that plumes have reached the upper plate. It was found empirically that  $t_p$ , scaled by the thermal diffusion relaxation time  $\tau_D$ , could be expressed as  $t_p/\tau_D = F([Ra - Ra_c])$ , where  $Ra_c$  is the critical Rayleigh number<sup>1</sup>. A model is proposed which reproduces this observed scaled representation. It uses the instability criterion of the bottom (hot) boundary fluid layer and the calculated Nusselt and Ra numbers for the steady-state convection. The perturbations leading to the convection development, after the fluid instability point has been reached, are unknown. Therefore  $t_p/\tau_D$  is determined within a constant multiplicative factor, the only fit parameter of this model. There is then good agreement over more than four orders of magnitude of  $[Ra - Ra_c]$  between the calculations and the experiments. The fit parameter is a phenomenological measure for the effectiveness of the perturbations, and will be discussed. 1. A. Furukawa et al. Phys. Rev. E 68, 056309 (2003), Fig.5a.

#### 3:30PM D8.00006 The Resolution of the Domain Chaos Puzzle for Rotated Rayleigh-Bénard

**Convection**<sup>1</sup>, NATHAN BECKER, GUENTER AHLERS, UC Santa Barbara — Due to the Küppers-Lortz instability, Rayleigh-Bénard convection-patterns exhibit spatio-temporal chaos at the onset of convection when the sample rotates fast enough about a vertical axis. Previous work showed that the scaling of the correlation length  $\xi$  determined from the experimental chaotic patterns disagreed with the prediction from a Ginzburg-Landau weakly-nonlinear model.<sup>2</sup> Commonly the power spectrum of the pattern images (the structure factor) is used to extract  $\xi$  from the half-width of its peak. Past experiments and simulations used standard Fourier techniques to calculate the power spectrum. On the basis of simulations using the Swift-Hohenberg equation, we show that those results are influenced strongly by the finite image-size available from experiment. The disagreement between experiment and theory was resolved by using the maximum-entropy method to calculate the power spectra. The maximum-entropy method is not as sensitive to the finite image-size effect. When applied to new experimental images, it yielded results for  $\xi$  that were in agreement with the theory.

<sup>1</sup>Work supported by NSF Grant DMR02-43336

<sup>2</sup>Y.-C. Hu, R. Ecke, and G. Ahlers, Phys. Rev. Lett. **74**, 5040 (1995).

3:42PM D8.00007 Revealing the building blocks of chaos: Deviations from extensivity , DAVID A. EGOLF, Dept of Physics; Georgetown University, MATTHEW P. FISHMAN, Dept of Physics; Georgetown University & Medical College of Wisconsin — Researchers have made relatively little progress in developing a predictive theory of far-from-equilibrium, spatially-extended chaotic systems. Even descriptions of the fundamental degrees of freedom and the nature of their interactions — central elements of statistical mechanics — are lacking. Using high- precision studies of the fractal dimension as a function of system length for the complex Ginzburg-Landau equation, we have uncovered deviations from extensivity on a length scale consistent with the chaotic length scale, indicating that this spatiotemporal chaotic system is composed of weakly-interacting building blocks, each containing about two degrees of freedom. Our results also suggest an explanation of some of the 'windows of periodicity' found in spatiotemporal systems of moderate size.

#### 3:54PM D8.00008 Estimating the State of Large Spatio-Temporally Chaotic Systems: Application to a Rayleigh-Benard Convection Experiment, MATTHEW CORNICK, EDWARD OTT, BRIAN HUNT, University of Maryland — Data Assimilation (DA) refers to the estimation of a dynamical system's state from the combined knowledge of past observations (possibly incomplete and noisy) and knowledge of an approximate model for the systems time evolution. Here we consider DA for spatio-temporally chaotic systems, and, in particular, we study the Local Ensemble Kalman Filter DA technique. We have applied this technique to Rayleigh-Benard convection undergoing spiral defect chaos. Using a system model (Boussinesq equations) and time series of noisy shadowgraphs we obtain estimates of the temperature and velocity field everywhere in a convection cell. This technique provides us with an indirect measurement of quantities previously inaccessible such as mean flow. We also demonstrate the utility of this method for forming initial conditions and producing 'forecasts' from the model.

#### 4:06PM D8.00009 Competition between left and right spiral vortices and their combinations

with different or equal amplitudes , MANFRED LÜCKE, ALEXANDER PINTER, CHRISTIAN HOFFMANN, University Saarbrücken — Stability, bifurcation properties, and the spatiotemporal behavior of different nonlinear combination structures of spiral vortices in the counter rotating Taylor-Couette system are investigated by full numerical simulations and by coupled amplitude equation approximations. Stable cross-spiral structures with continuously varying content of left and right spiral modes are found. Their solution provides a stability transferring connection between the initially stable, axially counter propagating wave states of pure spirals and the axially standing waves of so-called ribbons that become stable slightly further away from onset of vortex flow.

#### 4:18PM D8.00010 An Accurate Mode Selection Mechanism for Magnetic Fluids, DAVID JACKSON,

Dickinson College, JOSÈ MIRANDA, Universidade Federal de Pernambuco — When a ferrofluid is trapped in a Hele-Shaw cell and subjected to a perpendicular magnetic field a fingering instability results in the droplet evolving into a complex branched structure. This fingering instability depends on the magnetic field ramp rate but it also depends critically on the initial state of the droplet. Small perturbations in the initial droplet can have a large influence on the resulting final pattern. By simultaneously applying a stabilizing azimuthal magnetic field, we gain more control over the mode selection mechanism. In fact, a linear stability analysis predicts that any mode can be selected by appropriately adjusting the strengths of the applied fields. We present the results of numerical simulations that demonstrate that this mode-selection mechanism is quite robust and "overpowers" any initial perturbations on the droplet. This provides a predicable way to obtain patterns with any number of fingers whatsoever.

4:30PM D8.00011 Controlling Interfacial Instabilities in Hele-Shaw Cells: Theory, SHUWANG LI, JOHN LOWENGRUB, University of Califormia at Irvine, JAKE FONTANA, PETER PALFFY-MUHORAY, Liquid Crystal Institute, KSU — The growth of crystals in an undercooled melt and interface evolution in Hele-Shaw cells are governed by similar underlying mathematics. Hele-Shaw experiments can therefore give valuable insights into crystal growth. In the context of crystal growth, Li, Lowengrub and co-workers have demonstrated (e.g. see J. Crystal Growth, Physica D) that by varying the temperature conditions in the far-field in a prescribed way without feedback, interface instabilities (e.g. Mullins-Sekerka) can be suppressed and crystals may be grown with desired symmetries. Interestingly, at long times nonlinear stabilization is observed and leads to the existence of universal crystal shapes that depend only on the far-field temperature conditions. Here, this work is adapted to interface evolution in Hele-Shaw cells where the control parameter is the injection pressure. Namely, we consider the displacement of oil by air and we demonstrate that by varying the injection pressure in a prescribed, time-dependent way (without feedback) that the Saffman-Taylor instability can be suppressed and controlled such that bubbles of desired symmetries can form. This is in agreement with recent experimental predictions (presented separately in this session). We further predict the existence of universal bubble shapes that depend only on the injection pressure; the experimental confirmation of such universal shapes is the subject of ongoing studies.

4:42PM D8.00012 Controlling Interfacial Instabilities in Hele-Shaw Cells: Experiments , JAKE FONTANA, Liquid Crystal Institute, KSU, PETER PALFFY-MUHORAY, Liquid Crystal Institute, KSU, SHUWANG LI, University of California at Arvine, JOHN LOWENGRUB, University of California at Arvine, LIQUID CRYSTAL INSTITUTE TEAM, UNIVERSITY OF CALIFORNIA AT ARVINE TEAM — The growth of crystals in an undercooled melt and interface evolution in Hele-Shaw cells are governed by similar underlying mathematics. Hele-Shaw experiments can therefore give valuable insights into crystal growth. We have constructed radial Hele-Shaw cells where oil between parallel glass plates could be displaced by air whose injection pressure is a function of time. Here we describe our experimental apparatus and present results for the interface evolution for different driving schemes. We have found that, in agreement with recent theoretical predictions (presented separately in this session), we can prevent the onset of the Saffman-Taylor instability, or we can select and grow a particular unstable mode and drive the interface towards a corresponding universal shape. Varying the injection pressure during growth thus allows control over interfacial instabilities.

**4:54PM D8.00013 Liquid manipulation via morphological transitions**<sup>1</sup>, RALF SEEMANN, MARTIN BRINKMANN, EVGENY GUREVICH, STEPHAN HERMINGHAUS, MPI for Dynamics and Self-Organization, D-37073 Goettingen, JEAN-CHRISTOPHE BARET, MICHEL DECRE, Philips Research Laboratories, NL-5656AA Eindhoven — Liquid deposited on rectangular grooves, has a variety of possible liquid morphologies determined by the contact angle,  $\theta$ , and the exact channel geometry. In our experiments, electrowetting is used to tune  $\theta$  reversibly from 100 to 50 °, leading to a reversible transition between a drop- like morphology at large  $\theta$  and extended liquid filaments for small  $\theta$ . The transition is capillarity-driven but the behavior of the liquid above the transition is influenced by the electrical properties of the liquid. The static length of the liquid filament is a function of the applied Voltage and is in perfect agreement with a simple transmission-line model. Emphasis is put on the dynamic aspects of the filling and the draining behavior that follow a modified Washburn law. In case of thin and elastic ridges separating two grooves the cross talk of the liquid morphologies with the elastic substrate has an ordering effect on the position of the droplets.

 $^{1}$ This work was partly funded by the German Science Foundation under grant number SE1118 within the priority program Nano- and Microfluidics SPP 1164.

#### 5:06PM D8.00014 Diffusion-induced spontaneous pattern formation on gelation surfaces, HIROAKI

KATSURAGI, University of Pennsylvania, Kyushu University — Polymer gels make various kinds of surface patterns, which are typical non-equilibrium phenomena, under the volume phase transition. Mechanical instabilities due to swelling or shrinking of polymer gels play an essential role in such pattern formations. However, there is no report on diffusion-induced spontaneous pattern formation in polymer gels. Here we report the diffusion-induced (not caused by the mechanical instability) macroscopic pattern formation on gelation surfaces. We experimented on two-dimensional poly-acrylamide gelation that is governed by free radical polymerization. Gel slabs were made on Petri-dishes with free upper surface boundary condition. Then, random and straight stripe patterns (surface deformations) were observed, depending on gelation conditions. We consider a reaction-diffusion system. We found the scaling relation between the characteristic wavelength and the gelation time. This scaling is consistent with the reaction-diffusion dynamics.

5:18PM D8.00015 Using Capillary Flows to Pattern Lines<sup>1</sup>, SAURABH VYAWAHARE, KATE CRAIG, AXEL SCHERER, California Institute of Technology, Pasadena CA 91125 — One can appreciate how capillary forces cause unexpected patterns and shapes by looking at a soap bubble. Pattern formation by surface tension is seen in ring patterns of coffee stains, fingering patterns in Hele-Shaw cells, ordering of two dimensional micro-sphere crystals, combing of DNA and skeleton formation in marine creatures called radiolarians. Though comman, problems involving the understanding and control of the self-assembly mechanism need to be resolved before using capillary forces as a practical lithographic tool. Here, we report capillary flows create line patterns in evaporating liquids between closely spaced parallel plates. The widths of these lines range from a few microns to a few nanometers. Deliberate patterning of such lines requires pinning of the contact line and the presence of foaming surfactants. The position and type of line can be controlled with artificial pinning points and varying solutes respectively, and large-scale photolithography can be used to guide and control the definition of nanostructures. We provide "proof of principle" demonstrations of this method's application by creating lines of colloidal quantum dots and micro-spheres. This represents the first step in using capillary phenomena to create controlled, self-assembling, one-dimensional wire-like structures

<sup>1</sup>Support from the DARPA Optofluidics center is acknowledged

## Monday, March 13, 2006 2:30PM - 5:18PM -

Session DŽ1 DFD: Colloids III: Particles at Interfaces and in Confined Geometries Baltimore Convention Center 318

2:30PM D21.00001 Phase behavior of standing disks in 2D , KUN ZHAO, Princeton University, CHRISTOPHER HARRISON, Schlumberger-Doll Research Center, MATTHEW SULLIVAN, Princeton University, THOMAS MASON, University of California- Los Angeles, DAVID HUSE, WILLIAM RUSSEL, Princeton University, PAUL CHAIKIN, New York University — We use photolithography to fabricate plate-like colloidal PMMA disks (diameter~5.3micron, thickness~0.8micron). Using an electric field normal to the cover slip, we can get a monolayer of disks standing on their edges. The system resembles a 2D set of colloidal rectangles. We study the phase behavior of this system and find that there is K-T transition from isotropic to nematic (quasi-smectic). Between these two phases, we find a regime where tetratic correlations are longer range than nematic. By studying the disclinations and domain walls, we suggest that the tetratic phase is driven by the nearby nematic and exists on a length scale larger than the nematic domain wall spacing but smaller than the interdisclination distance.

2:42PM D21.00002 Attraction between charged silica spheres at a water-air interface<sup>1</sup>, PENGER TONG, WEI CHEN, Department of Physics, Hong Kong University of Science & Technology, SUSHENG TAN, WARREN T. FORD, Department of Chemistry, Oklahoma State University — Charged colloidal particles at aqueous interfaces are found to experience attractive interactions but the origin of such attraction is not well understood. Here we report an experimental study of attractive interactions between micron- sized charged silica spheres at a water-air interface. Atomic force microscopy is used to examine the charge distribution of the silica surface. Digital video microscopy is used to measure the equilibrium pair potential between the interfacial silica spheres over varying salt concentrations in the aqueous phase. It is found that the measured interaction potential U (r) has an energy barrier with height ~ 0.15  $k_BT$  at large particle separation r. For smaller separations, U(r) has an attractive well of order  $0.3k_BT$ . At even smaller separations, the usual Coulomb repulsion dominates. The experimental observation can be explained in terms of a balance between the screened Coulomb repulsion and unscreened dipole interactions.

<sup>1</sup>Work supported in part by the Research Grants Council of Hong Kong SAR under Grant No.

2:54PM D21.00003 Like-charge attraction originated from intrinsic charge inhomogeneity, YI ZHOU, ZHOUSHEN HUANG, TAI KAI NG, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, HongKong — We study attractions between charged colloidal spheres in a solution and at a water-air interface. Both intrinsic inhomogeneous charge distribution and induced charge fluctuations may result in like-charge attraction. The intrinsic inhomogeneous charge distribution comes from the inhomogeneous surfaces of colloidal spheres, characterized by the number of patchy domains, while charge fluctuations occur in a homogenous background of charges. As the number of patchy domains increases, it will change from the intrinsic charge inhomogeneity to the induced charge fluctuation case. This crossover is studied theoretically and the results are compared with the recent experiments on polystyrene and silicon particles. A simple mechanism is presented to explain the enhancement of the attraction between two charged colloidal particles when they are suspended near a wall.

**3:06PM D21.00004 Attraction between charged colloidal spheres at oil-water interface**, CHUAN ZENG, HUGO BISSIG, ANTHONY DINSMORE, Department of Physics, University of Massachusetts Amherst — The behavior of micron-sized, charged-stabilized colloidal spheres confined at oil-water interface was studied using microscopy. Aggregates of colloidal particles were observed, suggesting an attractive capillary force arising from electrostatic stress on the interface. We report measurements of a long-range attraction between carboxyl-modified polystyrene spheres (radius  $\sim 1$  micron) at the interface between 1,1,1-trifluoroheptan-2-ol and water using image analysis and particle tracking. The interaction between two isolated spheres was measured and compared to recent theoretical models. We also measured the interaction of single particles with large clusters as well as the interactions between clusters. We found acceleration due to the capillary attraction and a complex angular dependence owing to the anisotropy of the meniscus around a cluster. We acknowledge support from NASA through the Fluid Physics program (NRA 02-OBPR-03-C).

**3:18PM D21.00005** The elasticity of nanoparticle networks on liquid droplets , YOUNG-HSYANG CHEN, HSUAN-YI CHEN, Department of Physics, National Central University, Taiwan, ALEX LEVINE, Department of Chemistry and Biochemistry, University of California, Los Angeles, California — Inspired by recent experiments on the formation of linked nanoparticle networks [A.D. Dinsmore et al Science, 298, 1006, (2002)] on the surface of oil-in-water droplets, we study the modification of the droplet surface elasticity due to the formation of a percolating network of linked nanoparticles. What coverage of nanoparticles is required to modify the elasticity of the droplet? Using Brownian dynamics simulations to model the DLCA (diffusion limited cluster aggregation) of nanoparticles on the surface we construct these networks and monitor the appearance of an elastic contribution due to the nanoparticles at a critical nanoparticle area density. This transition is a type of rigidity percolation on a compact surface.

 $3:30PM D21.00006 Crystalline Particle Packings on Spheres^1$ , YAPING JING, Iowa State University, ALEX TRAVESSET, Iowa State University and Ames lab — The problem of packing particles on spheres appears in several soft condensed matter systems such as the building of PMMA cages (Pickering emulsions or colloidosomes), the micropatterning of colloidal particles relevant for photonic crystals or the geometric structures of Clathrin cages responsible for the vesicular transport of cargo in cells, just to name a few. In this talk we show how the structural and mechanical properties of spherical crystals can be described analytically from continuum elastic models and discuss how the results are extended to describe other geometries as well.

<sup>1</sup>funded by NSF-DMR-0426597

3:42PM D21.00007 A 3d View of Spherical Crystals and Grain Boundary Scars , MARK BOWICK, Syracuse University, THOMAS EINERT, PETER LIPOWSKY, JORG SCHILLING, ANDREAS BAUSCH, Technical University of Munich — We present an experimental system suitable for producing spherical crystals and for observing the distribution of lattice defects (disclinations and dislocations) on a significant fraction (50%) of the sphere. The introduction of fluorescently labeled particles enables us to determine the location and orientation of grain boundary scars. We find that the total number of scars and the number of excess dislocations per scar agree with theoretical predictions and that the geometrical centers of the scars are roughly positioned at the vertices of an icosahedron.

3:54PM D21.00008 Formation of nanoparticle-coated liquid metal droplets and measurement of their electronic properties.<sup>1</sup>, KAN DU, C. KNUTSON, RUI HONG, M. TUOMINEN, T. EMRICK, T. RUSSELL, A. DINSMORE, University of Massachusetts Amherst — We form stable droplets of molten metal, investigate their stability, and demonstrate their potential for forming electronic devices. Droplets of liquid Ga, 0.1-100 microns in diameter, were stabilized by surfactants and by insulating, conducting, and semiconducting nanoparticles. We investigate electronic transport through the nanoparticle-coated droplets. Here we use silica, gold and CdSe nanoparticles which spontaneously form a layer on the droplets. A few droplets form junctions between two platinum wires; we apply a bias voltage to the wires and measure the current before and after evaporation of the solvent. Improved understanding of the electrical characteristics may allow inexpensive assembly of a large number of devices with controlled size, symmetry and function. We acknowledge support from the Center for UMass/Industry Research on Polymers (CUMIRP).

<sup>1</sup>Center for UMass/Industry Research on Polymers (CUMIRP)

4:06PM D21.00009 MR Colloid Self-Assembly in Confined Geometries , PATRICK DOYLE, RAMIN HAGH-GOOIE, MIT — The characteristic length scales found in microfluidic devices have been shrinking drastically over the past several years. As a result it is becoming increasingly important to study the effects of this tight confinement. We have used the Brownian Dynamics simulation technique to study the self-assembly of magnetorheological (MR) colloids under confinement. To compliment these simulations, we have used particle tracking to study micron-sized colloids assembling in fluidic channels. For quasi-two dimensional systems, we report a seemingly contradictory response of the system to confinement between parallel hard walls. In contrast to previous circular geometries, we see re-entrant melting with respect to changing channel width and not with respect to field strength. As the channel height is increased (in the range of a few particle diameters), we observe oscillations in the mean cluster spacing with respect to gap height. These oscillations and the transition to the large gap scaling regime will be discussed.

4:18PM D21.00010 Confocal Microscopy of Hard Sphere Crystal Growth , MATTHEW SULLIVAN, Princeton University / Schlumberger-Doll Research, KUN ZHAO, ANDREW HOLLINGSWORTH, P.M. CHAIKIN, Princeton University / New York University, WILLIAM B. RUSSEL, Princeton University — Classical crystal growth is determined by the competition between chemical potential differences and surface tension. We use confocal microscopy to measure three dimensional crystal growth in a density matched suspension of PMMA-PHSA colloidal particles. The crystal is nucleated from a surface template that forces growth of face-centered-cubic crystals. The growing crystal surface is rough on the scale of several particle diameters, but the average growth rate is well described by the classical Wilson-Frenkel growth law. The local growth rate does depend on the roughness of the surface, however, and this growth rate variation provides a measure of interfacial surface tension.

4:30PM D21.00011 Simulated Crystallite Melting Kinetics in Two Dimensions, D. W. BLAIR, J. R. SAVAGE, A. D. DINSMORE, J. MACHTA, R. A. GUYER, University of Massachusetts at Amherst, A. J. LEVINE, University of California, Los Angeles — We report on results of numerical simulations of the melting of two-dimensional crystallites. Recent experiments in colloidal systems demonstrate that colloidal crystallites undergo a two-stage melting process. Initially large crystallites melt at a constant rate until reaching a critical size at which there is a dramatic increase in the melting rate. Throughout the initial melting stage the crystallite interior maintains bond orientational order; this order is abruptly lost at the critical size. Using Brownian dynamics simulations of particles interacting via a variety of short-range central potentials, we find that in two dimensional order. The critical size, particle number O(20), is in agreement with experimental data and appears insensitive to details of the short-range interparticle potential. We discuss a possible mechanism for this change in melting dynamics at a critical crystallite size. This work is supported in part by NSF (DMR-0242402) and NASA (NAG8-1659).

4:42PM D21.00012 Influence of hydrodynamic coupling on pair-diffusion in a quasi-onedimensional colloid system<sup>1</sup>, BINHUA LIN, XINLIANG XU, STUART RICE, University of Chicago, HAIM DIAMANT, Tel Aviv University — The effect of hydrodynamic interaction on the separation dependence of the center of mass and relative pair diffusion coefficients of colloid particles in a quasi-one-dimensional system, including the influence of proximate walls, has been calculated using the method of reflections. There is excellent agreement between the theoretical predictions and the experimental data. We show that the separation dependence of the relative pair diffusion coefficient has oscillatory structure on the scale length of the correlation length in the system, and we directly relate that oscillatory structure to the pair correlation function of the system.

<sup>1</sup>This research was supported by grants from the NSF (CHE-0241133, CTS-021774).

4:54PM D21.00013 Short-time dynamics of a Brownian particle , BRANIMIR LUKIC, Ecole Polytechnique Federale de Lausanne (EPFL), Switzerland, SYLVIA JENEY, ZELJKO SVIBEN, EPFL Lausanne, CHRISTIAN TISCHER, EMBL Heidelberg, Germany, ERNST-LUDWIG FLORIN, Center for Nonlinear Dynamics, University of Texas, Austin, ANDRZEJ J. KULIK, LASZLO FORRO, EPFL Lausanne — We record the thermal position fluctuations of a *single* micron- sized sphere immersed in a fluid by optical trapping interferometry with nanometer spatial and microsecond temporal resolution. On the shortest time scales investigated, the sphere's inertia has a small, but measurable, effect. We find, in accord with the theory of Brownian motion including hydrodynamic memory effects, that the transition from ballistic to diffusive motion is delayed to significantly longer times than predicted by the standard Langevin equation. This delay is a consequence of the inertia of the fluid. When the particle is confined by a harmonic potential with observe the free diffusive behavior in such confined system.

5:06PM D21.00014 Transport of nanoparticles in a temperature gradient, shawn putnam, david CAHILL, Center of Advanced Materials for the Purification of Water with Systems, Univ. of Illinois — Thermodiffusion, mass transport in a temperature gradient, is commonly characterized by either the thermodiffusion coefficient  $D_T$  or the Soret coefficient  $S_T$ ; e.g., allow particle concentration c, the particle flux of a colloidal suspension subjected to a temperature gradient  $\nabla T$  is  $\mathbf{J} = -cD_T\nabla T - D_c\nabla c$ , where  $D_c$  is the diffusion coefficient and the Soret coefficient is  $S_T = D_T/D_c$ . We present our measured  $D_T$  data for aqueous suspensions of charged polystyrene spheres, alumina nanoparticles, and globular proteins of lysozyme. Special emphasis is given to our published work on charged polystyrene spheres with different surface functionalities. For example, in solutions with large concentrations of monovalent salts,  $\gtrsim$  100 mM,  $D_T$  for 26 nm spheres with carboxyl functionality can be varied within the range  $-0.9 \times 10^{-7}$  cm<sup>2</sup> s<sup>-1</sup>  $K^{-1} < D_T < 1.5 \times 10^{-7} \text{ cm}^2 \text{ s}^{-1} \text{ K}^{-1}$  by changing the ionic species in solution; in this case  $D_T$  is the product of the electrophoretic mobility  $\mu_E$  and the Seebeck coefficient of the electrolyte  $S_e = (Q_C^* - Q_A^*)/2eT$ ,  $D_T = -S_e \mu_E$ , where  $Q_C^*$  and  $Q_A^*$  are the single ion heats of transport of the cationic and anionic species respectively. On the contrary, in low ionic strength solutions of LiCl,  $\leq 5 \text{ mM}$ ,  $D_T$  for the 26nm carboxyl spheres is negative, independent of particle concentration, and independent of the Debye length;  $D_T = -0.73 \pm 0.05 \times 10^{-7}$  cm<sup>2</sup> s<sup>-1</sup> K<sup>-1</sup>. The temperature dependence of  $D_T$  is also discussed with results from our current work with polystyrene spheres, alumina nanoparticles, and protein solutions of lysozyme.

## Tuesday, March 14, 2006 8:00AM - 10:48AM – Session G8 DFD GSNP: Patterns and Instabilities II Baltimore Convention Center 314

8:00AM G8.00001 Dynamics of Swarms, NICHOLAS MECHOLSKY, EDWARD OTT, TOM ANTONSEN, University of Maryland Deptartment of Physics — The collective behavior of animal groups (swarms, herds, flocks, etc.) provides a fascinating instance of a self-organizing system. In this poster we consider continuum model descriptions of animal groups with particular emphasis on dynamics and relaxation of the collective behavior of such groups. Topics considered will include equilibrium swarms, waves on swarms, relaxation to equilibrium, excitation of waves by obstacles and predators, and

8:12AM G8.00002 Drying Mediated Pattern Formation in a Capillary-Held Polymer Solution<sup>1</sup>, ZHIQUN LIN, JUN XU, SUCK WON HONG, JIANFENG XIA, Materials Science and Engineering Department, Iowa State University, Ames, IA 50011 — We demonstrated that concentric ring patterns of high regularity could form spontaneously, simply by allowing a droplet to evaporate in a consecutive "stick-slip" motion in a confined geometry. The process resembled neatly stacked rows of driftwood abandoned by receding tides. The use of solutions with different concentrations and different solvents effectively mediated the evaporative loss of the solvent and the deposition time of the solute, thereby affecting the centerto-center distance between adjacent rings and the height of the ring. A theoretical calculation based on the mass conservation of the solution has, for the first time, been performed to reveal the nature of the formation of gradient ring patterns in a confined geometry. The studies demonstrate that dynamic self-assembly in a confined geometry may offer a new approach to produce gradient features, as well as a simple, versatile, generalizable approach to produce yet more complex patterns. This natural, pattern-forming process could find use in the fields such as nanotechnology and optoelectronics.

<sup>1</sup>Acknowledgement: ISU startup, ISU University Research Grant, and ACS-PRF

8:24AM G8.00003 A network model of channel competition in fracture dissolution<sup>1</sup>, TONY LADD, University of Florida, PIOTR SZYMCZAK, Warsaw University — During dissolution in porous or fractured rock, a positive feedback between fluid transport and chemical reactions at the mineral surfaces may lead to the formation of pronounced, wormhole-like channels. As the dissolution proceeds the channels interact, competing for the available flow, and eventually the growth of the shorter ones ceases. Thus the number of channels decreases with time while the characteristic distance between them increases, which leads to a scale-invariant, power-law distribution of channel lengths. A simple resistor network model of the evolution of dissolving channels is constructed and its properties studied. The results are compared with pore-scale simulations of fracture dissolution using a microscopic, three-dimensional numerical model. Despite its simplicity, the resistor model is found to retain the essential features of the nonlinear interaction between the channels.

<sup>1</sup>This work was supported by the US Department of Energy, Chemical Sciences, Geosciences and Biosciences Division, Office of Basic Energy Sciences (DE-FG02-98ER14853), and by the Polish Committee of Scientific Research (P03B 08127, 2004-2005)

8:36AM G8.00004 Fractal growth of liquid crystals as a hysteresis phenomenon, HO-KEI CHAN, INGO DIERKING, School of Physics and Astronomy, University of Manchester, Manchester (U. K.) — Fractal percolation growth of liquid crystal phases within a supercooled isotropic liquid medium has been observed in recent years. Notable examples include the B2 phase of 'banana' mesogens [1] and the smectic C phase of a calamitic hydrogen-bonding liquid crystal [2]. Here we present a dynamical model that describes such fractal growth as well as the spherical growth conventionally observed for nematics and cholesterics. The essential idea is that the supercooled medium does not fully respond to the temperature quench immediately (hysteresis). Its fraction of space available for the phase transition only relaxes from 0 to 1 at some finite rate. Depending on the coupling between the relaxation and growth rates, the liquid crystal phase either grows as a percolation cluster of fractal dimension  $D \approx 1.89$  or approaches a spherical shape of Euclidean dimension  $D \rightarrow 2$ . The crossover behaviour from relatively slow to fast relaxation is thoroughly investigated. Possible causes of the hysteresis for fractal growth will be discussed.

[1] I. Dierking, Liq. Cryst. Today 12(1), (2003), 1

stability.

[2] I. Dierking, Chan H. K., Culfaz F., McQuire S., Phys. Rev. E 70, (2004), 051701

8:48AM G8.00005 Patterns in type-I superconductors and their dynamics, RINKE J. WIJNGAARDEN, MARIELA MENGHINI, Department of Physics and Astronomy, Faculty of Sciences, Free University, De Boelelaan 1081, 1081 HV Amsterdam, The Netherlands - We report on patterns and their dynamics as observed in magneto- optical experiments on type-I superconductors. We observe: (1) A stripe-spot transition that is hysteretic, leading to two modes of stripe formation: slow continuous growth and avalanche growth. (2) A wiggling instability, similar to that in ferrimagnetic garnet films. (3) A zigzag instability when a pattern of parallel lines is rotated through a sample with low pinning. (4) Breaking and reconnection of stripes as such a pattern is rotated in a sample with strong pinning. (5) Random telegraph behavior close to the depinning of such pattern in the presence of a constant driving force. The observed patterns consist of superconducting and normal domains of macroscopic size in thin lamina of type-I superconductors and are observed by an advanced magneto-optical technique. The patterns are manipulated by changing the applied magnetic field vector or by applying an electrical transport current.

9:00AM G8.00006 Scaling in activated escape of underdamped systems , IRA SCHWARTZ, Naval Research Laboratory, MARK DYKMAN, MICHAEL SHAPIRO, Michigan State University — Noise-induced escape from potentials is ubiquitous in many areas of physics. Here, noise-induced escape from a metastable state of a dynamical system is studied close to a saddle-node bifurcation point, but in a region where the system remains underdamped. We find the activation energy of escape scales as a power of the distance to the bifurcation point. Moreover, we find two types of scaling and the corresponding critical exponents.

9:12AM G8.00007 The Analysis of Spatiotemporal Chaos in Very Large Data Sets Generated by Electroconvective Experiments with Nematic Liquid crystals<sup>1</sup>, JOSHUA LADD, Colorado State University, GYANU ACHARYA, Kent State University, J.T. GLEESON, Kent State University — Spatiotemporal chaos (STC) has been empirically observed in electrohydrodynamic convection in a planar layer of the nematic liquid crystal I52. The observed spatiotemporal dynamics is due to the interaction of two families of counter propagating waves that loose stability at onset. Thus it is possible to describe the patterns through a system of Ginzburg –Landau equations that governs the evolution of the envelopes of these waves (*Denin et al, Science 1996*). In this work we extract the envelopes from spatiotemporal data generated by electroconvective experiments done at Kent State University using a demodulation procedure. Once obtained it is possible to separate spatial and temporal components of the dynamics by employing the singular value decomposition. This is done in order to study the chaotic nature of the pattern. Comparison is made with numerical STC obtained from computer simulations of the Ginzburg-Landau system derived from the weak electrolyte model (*Dangelmayr & Oprea, 2002*) of electroconvection.

<sup>1</sup>Supported by NSF-DMS 0407418

**9:24AM G8.00008 Pattern formation in liquids under unipolar space charge injection**<sup>1</sup>, FRANCISCO VEGA REYES, Departamento de Fisica, Universidad de Extremadura, E-06071 Badajoz, Spain, FRANCISCO J. GARCIA, Departmento de Fisica Aplicada I, EUITA, Universidad de Sevilla, Spain — We study experimentally the hydrodynamic stability of thin liquid layers subjected to corona discharge in the air. We obtain clear direct images and movies of the observed hydrodynamic instabilities and patterns. After this we apply an image processing method that allows us to quantify the liquid interface deformation. We use a variety of liquids whose properties may differ in orders of magnitude. Particularly, we use series of liquids with different electric conductivity or viscosity while keeping constant the rest of the properties. In this way, we can track quantitatively the instabilities as a function of only one of these properties. This, together with our image processing method, allows us to study and classify the different instabilities. The peculiar properties of the electric field in the liquid interface when there is a space charge injection have not been studied until very recently. Results show clearly the influence (and relevancy) that the properties of this electric field have in the formation (or not) of the different patterns observed when the liquid properties are varied.

<sup>1</sup>This work was supported by the Spanish Ministry of Education and Science under research project BFM-2003-01739.

9:36AM G8.00009 Path stability of a rising bubble<sup>1</sup>, BINZE YANG, ANDREA PROSPERETTI, Johns Hopkins University — A millimeter-size gas bubble rises in a zigzag or spiral path in still water. A linear analysis of this process is presented assuming that the bubble has a fixed ellipsoidal shape of varying aspect ratio. The results exhibit a strong similarity to the stability features of the flow past a solid sphere. By focusing on the m= 1 azimuthal mode, it is found that a double-threaded wake responsible for the deviation from the vertical path develops when the aspect ratio is sufficiently large. The stability analysis of "frozen" states before steady conditions are achieved shows that the amount of vorticity accumulated at the rear of the bubble plays an essential role for the instability. It is also shown that, in the common parameter ranges of interest, the instability is very sensitive to the deformation of the bubble, but relatively insensitive to the Reynolds number.

<sup>1</sup>Supported by NASA

9:48AM G8.00010 Flame Propagation with Hydrodynamic and Body-Force Instabilities , KUO-LONG PAN, Department of Mechanical Engineering, National Taiwan University — The hydrodynamic (Darrieus-Landau) instability is an intrinsic mechanism that wrinkles the flame surface. In the nonlinear stage, propagation of flame wrinkles can evolve to a quasi-stable state characterized by a solitary wave or chaotic form with corrugated front. The underlying structures, i.e. incessant merging of near wrinkles and creation of new cells, have been studied numerically. It reveals the significance of asymmetric perturbation in breaking the symmetry. The effect of gravity was also investigated. It was found that, while wrinkled flames can be stabilized by negative gravity of moderate magnitude, the wrinkles at short wavelength,  $\lambda$ , remains intact if the magnitude is small while those at long  $\lambda$  are suppressed. As such, compared to the zero-gravity state, diminishing multiplicity of cellular scales and subsequently decreasing interactions among the multi-scale wrinkles mollify the chaotic complication. When slight positive gravity is introduced, the unsteady evolution is suppressed. The somehow stabilizing effect, while in contrast to the destabilization at linear stage, is due to the coupling of D-L instability and Rayleigh-Taylor instability that prevents excitation of secondary D-L instability. If the magnitude is strong enough, however, the ordered pattern degenerates and highly irregular flame surface is formed without specific cell structure. This is a typical appearance of R-T instability caused by buoyancy.

10:00AM G8.00011 Numerical Simulation of Conductivity Gradient-Induced Electrokinetic Flow Instabilities, STEPHEN BRADFORD, UC Santa Barbara, CARL MEINHART, UC Santa Barbara, JON POSNER COLLABORATION, JUAN SANTIAGO COLLABORATION — This research is focused on the electrokinetic flow instabilities observed in long, thin microchannels with conductivity gradients orthogonal to the streamwise direction and applied potential. This situation often occurs in field amplified sample stacking (FASS) and isoelectric focusing, where control of the instabilities arise from fluid body forces generated by the action of applied electric fields on electrolyte concentration-based conductivity gradients. A model is developed to describe the phenomena in general and applied specifically to thin microchannels with the conductivity gradient perpendicular to the applied field (both DC and AC). A higher-order, depth averaged correlation is proposed to account for the out of plane effects. Numerical simulations performed using COMSOL 3.2 are compared to 2-D and 3-D simulations as well as experimental data for multiple geometries with good agreement.

10:12AM G8.00012 Particle production in non-dissipative shock-waves , ALEXANDER ABANOV, Stony Brook University, FABIO FRANCHINI — We study non-dissipative shock-waves in the effective hydrodynamics of some correlated one-dimensional integrable systems. The semiclassical dynamics of these systems is governed by integrable non-linear classical equations such as the Benjamin-Ono and the KdV equations. The development of non- dissipative shock-waves from a large disturbance of the fluid is described by Gurevich-Pitaevsky theory. The theory describes how the instability of a large disturbance of the fluid is resolved by producing oscillations which develop into a train of solitons at large times. We establish the connection between this classical picture and the production of quasi-particles in the underlying quantum system. The semiclassical (background) configuration can then be thought of as an effective metric in which these excitations move. This approach is done in the spirit of the original proposal of Unruh, who suggested to model the Hawking radiation from black holes by an emission of thermal sound waves from the sonic horizon in transsonic fluid flow.

10:24AM G8.00013 Torsional Motion of Rotating Particles with Graded Couplings , H.W. TSANG, J.J. XIAO, K.W. YU, The Chinese University of Hong Kong — Localization of excitations occurs in many physical systems. There are two common types of localization. The first type is a consequence of interference of coherent vibrational waves due to diffusive scattering like Anderson localization in lattice vibration. The other type of localization is due to confinement by impurities like defect modes. Graded systems occur in a variety of physical system. It is of great interest to analyze the localization of excitations in graded system [1]. In this work, we consider a system of rotating particles with graded torsional couplings. The steady-state solutions are solved directly from the dynamic equations. Energy is localized in the region of stronger couplings at high frequencies. A dynamic stimulation based on forced rotors is performed both for the graded linear and graded non-linear coupling potential subjected to a sinusoidal driving torque. In the small amplitude region, the results of non-linear potential are similar to those of the linear ones. The major difference is that the rotational amplitude is larger for the non-linear potential. Energy transfer may thus be more effective in the non-linear case. In the large amplitude region, chaos may occur and contribute to the localization.

[1] J. J. Xiao, K. Yakubo, and K. W. Yu, Harmonic vibrational excitations in graded elastic networks: transition from phonons to gradons, unpublished.

10:36AM G8.00014 Numerical simulations of inertial migration in a square duct: An investigation of multiple equilibrium positions<sup>1</sup>, BYOUNGJIN CHUN, University of Florida, TONY LADD — In Poiseuille flow, a neutrally-buoyant particle migrates to a position that is determined by the balance of forces generated by the gradient of the shear rate and interactions of the flow field with the container walls. In a cylindrical flow, uniformly distributed particles migrate to form a stable ring located at approximately 0.6 times the cylinder radius. However, recent experiments show two interesting new observations. First the suspended particles tend to align near the walls to make linear chains of more or less equally-spaced particles, and second, at high Reynolds numbers (Re 1000), an additional inner ring of particles is formed. The inner ring is only formed when the particle are large, of the order of 1:10 the cylinder diameter. We have used numerical simulations based on the lattice-Boltzmann method to investigate inertial migration of neutrally buoyant particles in a square duct over a range of Reynolds numbers from 100 to 1000. Our results show trains of particles being formed along the axis of the flow, near the planar equilibrium positions of single particles. At Reynolds number greater than 750, particles appear near the center of the duct as well. We will present a new mechanism to interpret and understand these results, which was discovered by examining the migration of single particles and rigid dumbbells.

<sup>1</sup>This work was supported by the National Aeronautics and Space Administration, NAG NNCO4GA89G.

#### Tuesday, March 14, 2006 8:00 AM - 11:00 AM $_-$

Session GŽ1 DFD: Colloids IV: Polymeric and Colloid-Polymer Systems Baltimore Convention Center 318

8:00AM G21.00001 Self Assembly of Temperature-Sensitive Capsules using PNIPAm Microspheres<sup>1</sup>, D. B. LAWRENCE, University of Massachusetts Amherst Physics, T. CAI, Z. B. HU, University of North Texas, M. MARQUEZ, INEST Group, Phillip Morris USA, A. D. DINSMORE, University of Massachusetts Amherst Physics — We present a method for self assembly of novel semi-permeable capsules (colloidosomes) exhibiting temperature-dependent size and surface properties. These hollow micro-capsules are composed of micron-sized PNIPAm-co-acrylic acid particles that exhibit a reversible size transition at 32°C. The PNIPAm particles self-assemble at the spherical interface between 2-Octanol and water droplets. Electrostatic cross-linking with the di-block copolymer Poly(butadiene-b-N-methyl 4-vinyl pyridinium iodide) locks the particles in place, forming a rigid, elastic membrane that remains after the 2-Octanol/Water interface is removed. Such self-assembled capsules retain the temperature sensitivity of the PNIPAm particles from which they are constructed, and exhibit reversible size transitions. Controlled variation of the permeability and potential applications in controlled release will be discussed.

<sup>1</sup>We acknowledge support from the Kraft Foods, Inc. NanoteK consortium.

8:12AM G21.00002 Femtonewton Measurements of Polymer-Mediated Colloidal Interaction , SVEN BEHRENS, BASF, HELMUT AUWETER, BASF — The stability of colloidal dispersions hinges on the repulsive interaction between the particle surfaces. This interaction can be modified by adsorbed polymer and further tuned by the response of the adsorbate layer to changes in the surrounding solution. Total internal reflection microscopy has been used in this study to investigate the effect of charged and neutral polymer adsorbates on the interaction of a colloidal particle with a flat substrate. The results were correlated with light scattering studies of the employed polymers in solution and of polymer-coated particles; they reveal a subtle interplay of steric, electrostatic, and van der Waals forces.

#### 8:24AM G21.00003 Phase Behavior of Charged Colloid-Polymer Mixtures: A Simulation

 $Study^1$ , BEN LU, ALAN R. DENTON, Department of Physics, North Dakota State University — We present a Monte Carlo simulation study of mixtures of charged colloids and nonadsorbing polymers. The multicomponent mixture of colloidal macroions, microions (counterions and salt ions), polymers, and solvent is modeled as an effective two-component mixture of pseudomacroions and neutral polymers. The pseudomacroions are assumed to interact via effective electrostatic interactions<sup>2</sup> (screened-Coulomb pair potential and one-body volume energy) and the polymers are treated as effective spheres that have hard interactions with the colloids but are mutually ideal. Previous studies have identified the volume energy as the driving force for phase separation of deionized colloidal suspensions<sup>3</sup> and polymer depletion-induced attraction as the origin of colloid-polymer demixing. Here we apply the Gibbs ensemble Monte Carlo method to the effective binary mixture to examine the combined influences of electrostatic and depletion-induced interactions on phase behavior.

<sup>1</sup>Support from the National Science Foundation (grant DMR-0204020) is gratefully acknowledged.

<sup>2</sup>A. R. Denton, *Phys. Rev.* E **62**, 3855 (2000).

<sup>3</sup>R. van Roij, M. Dijkstra, and J.-P. Hansen, Phys. Rev. E 59, 2010 (1999); P. B. Warren, J. Chem. Phys. 112, 4683 (2000).

8:36AM G21.00004 Demixing of Charged Colloid-Polymer Mixtures: Variational Theory<sup>1</sup>, SHRIKANT SHENOY, ALAN R. DENTON, Dept. of Physics, North Dakota State University — We investigate thermodynamic phase behavior of mixtures of charged colloids and neutral nonadsorbing polymers using a variational method for the free energy. The mixture of macroions, microions, and solvent is first mapped onto an effective one-component system of pseudomacroions that interact via effective electrostatic interactions. The polymers are modeled as effective spheres that have hard interactions with the colloids but are mutually ideal. The charged colloid-polymer mixture is then mapped onto an Asakura-Oosawa model with effective colloid and polymer diameters<sup>2</sup>. The free energy is approximated by combining thermodynamic perturbation theory for the colloids with free-volume theory for the polymers and minimizing with respect to the effective colloid diameter. Phase diagrams are computed by a coexistence analysis that ensures equality of pressures and of chemical potentials of all species in the two phases. The resultant phase behavior depends sensitively on colloid charge, polymer-to-colloid size ratio, and composition. Electrostatic repulsion between colloids is found to stabilize the mixture against polymer depletion-induced demixing, consistent with previous predictions<sup>3</sup> and experimental observations.

<sup>1</sup> Support from the National Science Foundation (grant DMR-0204020) is gratefully acknowledged.

<sup>2</sup> A. R. Denton and M. Schmidt, J. Chem. Phys. 122, 2449111 (2005).

8:48AM G21.00005 Preparation of PHSA-PMMA stabilizer for model hard sphere systems, ANDREW HOLLINGSWORTH, New York University, WILLIAM RUSSEL, Princeton University, CARLOS VAN KATS, ALFONS VAN BLAADEREN, Utrecht University — Sterically-stabilized colloidal particles are an excellent model hard-sphere system used by many groups. One of the original stabilizers used for such systems was developed and patented by ICI more than 30 years ago. It consists of a 'comb-like' stabilizer of a poly(12-hydroxystearic acid) which is soluble in aliphatic hydrocarbons. These pendant PHSA chains are grafted to an insoluble poly(methyl methacrylate) backbone that strongly adsorbs to polymer particles and thus provides a means of anchoring stabilizer to particle surfaces. Unfortunately, the PHSA-g-PMMA stabilizer is not commercially available. Furthermore, the three-step procedure (Antl, et al. 1986) is generally regarded by non-chemists as technique intensive and time-consuming. We have systematically studied the PHSA-PMMA stabilizer synthesis with the goal of taking the mystery out of the protocol and making the entire synthesis reproducible. Several important details, not published in the literature, will be discussed, along with the analytical results from mass spectroscopy, proton NMR, acid titration and gel permeation chromatography, all of which were used to characterize the polymer and its precursors.

9:00AM G21.00006 Self-assembly of Asphaltenes: Enthalpy, Entropy of Depletion and Dynamics at Crossover I-experimental, NATALIA LISITZA, DENISE FREED, PABITRA SEN, YI-QIAO SONG, Schlumberger-Doll Research — The continuous rise of global demand for energy and the difficulty of significantly increasing production have driven the petroleum industry to develop much more difficult oil reservoirs, such as deep-water fields. Asphaltenes, naturally-occurring large aromatic molecules in crude oils, are known to be the "cholesterol" of petroleum because they self-associate to form solid aggregates and eventually clog the production pipes and the rocks. An extraordinary amount of work using many analytical techniques has been applied to elucidate the properties of asphaltenes. However, many fundamental issues, such as the molecular architecture and the aggregation mechanisms, are still in debate. Here we use NMR to detect asphaltene aggregation in toluene solutions and to obtain both the enthalpy and entropy of this process. We observe an abrupt drop of the asphaltene diffusion constant which is indicative of a molecular conformation (shape) change. This change is intimately related to or possibly a prerequisite of the aggregation. The entropy of aggregation was found to be positive due to the excluded volume effect for the solvent. This is reminiscent of the depletion entropy force, which is considered to be the driving force for the aggregation of much large

9:12AM G21.00007 Self-assembly of Asphaltenes: Enthalpy, Entropy of Depletion and Dynamics at Crossover II - theoretical, DENISE FREED, NATALIA LISITZA, PABITRA SEN, YI-QIAO SONG, Schlumberger-Doll Research — NMR spin-relaxation is directly sensitive to molecular dynamics and is therefore an excellent tool for studying the formation of nano-aggregates. When aggregates form, the molecular rotations are slowed down, and the spin-relaxation rate is enhanced, which reduces the NMR signal. This gives rises to a remarkable kink in the NMR signal intensity at the Critical Nano-Aggregate Concentration (CNAC). In this talk, we use Debye's two-state model for micelle formation to describe asphaltene aggregation. We use the temperature dependence of the CNAC to determinate the enthalpy and entropy of aggregation. The enthalpy is negative, as expected, and indicates that the aggregate formation is energetically favorable due to  $\pi$ -stacking interactions. On the other hand, we find that the entropy is positive, which is quite a surprise. We propose that this increase comes from the depletion entropy of the solvent. As asphaltene molecules aggregate, the free volume available for the solvent molecules increases, giving rise to a depletion effect. An estimate of the depletion entropy from the sizes of asphaltene and toluene (solvent) is very close to the measured entropy gain. We will also discuss the applicability of Debye's two-state model to aggregate formation in asphaltene solutions.

#### 9:24AM G21.00008 Molecular Diffusivities of Asphaltene Monomers by Fluorescent Correla-

tion Spectroscopy , BALLARD ANDREWS, Schlumberger-Doll Research, RODRIGO GUERRA, Harvard University, PABITRA SEN, Schlumberger-Doll Research, OLIVER MULLINS, Schlumberger-Doll Research — Many analytical techniques have been applied to elucidate the properties of asphaltenes due to their extraordinary importance in the petroleum industry. However, many fundamental issues such as the molecular size are still in debate. Using Fluorescence Correlation Spectroscopy (FCS) we measure the translational diffusion coefficient of asphaltene molecules in toluene at extremely low dilutions. To avoid focal volume artifacts common in FCS we use a scaling procedure to determine asphaltene diffusivities relative to known molecules such as porphyrins, perylene and quantum dots. We estimate a diffusion coefficient for the asphaltene molecules of 0.3,  $10^{-5}$  cm<sup>2</sup>/sec at room temperature. This value agrees with recent estimates from NMR studied at 10-100 fold higher concentrations. The Stokes-Einstein equation implies that the unaggregated hydrodynamic diameter of asphaltene monomers is 15-25 Å.

9:36AM G21.00009 Novel emulsions stabilized by pH and temperature sensitive microgels, TO NGAI, The Chinese University of Hong Kong, HELMUT AUWETER, BASF, SVEN BEHRENS, BASF — Poly(N-isopropylacrylamide-co-methacrylic acid) (PNIPAM-MAA) microgel particles in aqueous solution exhibit a volume phase transition that can be induced by changes of either pH or temperature. In the swollen state, these microgels self-assemble at an octanol-water interface and can be used to stabilize surfactant-free oil-in-water emulsions. This stabilizing efficiency is retained even in the collapsed state, provided that the microgels are fully charged. At very low charge (low pH), on the other hand, the microgels migrate completely into the oil phase, and the emulsion breaks. In an intermediate regime of practical interest the emulsion stability can be tuned by small adjustments of pH or temperature. Because of this unprecedented stability control, we believe that such stimulus-responsive charged microgels have a great of both classical surfactants and solid particles.

#### 9:48AM G21.00010 Internal Dynamics of Double Emulsion Creams and Polymer-Dispersed

**Complex Droplets** , HU GANG, Hong Kong Baptist University — The availability of monodisperse double emulsions allows for detailed study of their stability and rheological properties. Practical use of double emulsions concerns the structure and structural evolution of the complex droplets. The usually achievable size of the complex droplets ranges from a micrometer to tens of micrometers. To obtain a homogeneous system, a double emulsion has to be in the form of cream or gel to avoid macroscopic phase separation. However, immobilizing the double emulsion drops does not cease the full dynamics since the internal smaller droplets are also subject to thermal agitation. The ability to track the evolution of the internal encapsulated phase is essential to the understanding of the kinetic stability of a new formulation. Conventional light scattering encounters significant difficulties to probe the structure of concentrated emulsions while diffusing-wave spectroscopy (DWS) shows a unique advantage. We prepare monodisperse W/O/W double emulsions and apply DWS to study the structure of double emulsion creams and gels. We also test the sensitivity of DWS when the amount of encapsulated phase is varied by induced coalescence or osmotic gradient.

10:00AM G21.00011 Quasi-two-dimensional equilibrium and non-equilibrium thermodynamics of thin liquid films stabilized by colloidal particles<sup>1</sup>, JERZY BLAWZDZIEWICZ, Yale University, ELIGIUSZ WAJNRYB, IPPT, Warsaw, Poland — Due to the presence of oscillatory structural forces, static and dynamic properties of thin liquid films stabilized by colloidal particles, or macromolecules differ from the properties of particle-free films. During drainage process, particle-stabilized films often form a stepwise structure with coexisting regions (phases) of uniform but different thickness. We describe film phase equilibria using a quasi-two dimensional thermodynamic formalism. The key quantity in our approach is the film tension. We show that the particle contribution to this quantity results from the anisotropy of the particle somotic-pressure tensor in the film. The quasi-2d description is also developed for non-equilibrium film states. We show that the motion of particle-stabilized films is analogous to the dynamics of a two-dimensional compressible fluid - the film thickness plays the role of mass density per unit area and film tension the role of pressure. In the linear-response regime, the film dynamics is characterized by the shear and extension viscosity coefficients. There are also two independent kinetic coefficients relating the particle flux to the gradients of the normal osmotic pressure and particle chemical potential. For a film stabilized by a suspension of hard spheres we have calculated these coefficients using a multipolar-expansion methods combined with a flow reflection technique.

<sup>1</sup>Supported by NASA grant NAG3-2704 and NSF grant CTS-0348175

#### 10:12AM G21.00012 Dynamics, Rectification, and Fractionation for Colloids on Flashing Sub-

strates , ANDRAS LIBAL, University of Notre Dame, CHARLES REICHHARDT, Los Alamos National Laboratory, BOLDIZSAR JANKO, University of Notre Dame, CYNTHIA OLSON REICHHARDT, Los Alamos National Laboratory — We show that a rich variety of dynamic phases can be realized for monoand bidisperse mixtures of interacting colloids under the influence of a symmetric flashing periodic substrate. These type of substrates have been attracting growing interest due to recent experimental breakthroughs that allow the creation of dynamic periodic arrays using optical and holographic techniques. With the addition of dc or ac drives, these system show phase locking, jamming, and new types of ratchet effects. We studied these effects in detail. The ratchet effect can be used for charge separation of a bidisperse system. In this system, in some regimes we find that the addition of a non-rathceting species increases the velocity of the ratcheting particles. We show that these effects occur due to the collective interactions of colloids. 10:24AM G21.00013 Formation of Extended Optical Traps by Shape-Phase Modulation - Measuring Inter-Colloidal Interactions in Tailored Potential Landscapes, YOHAI ROICHMAN, DAVID G. GRIER, Soft Matter Research Center, Physics dept., New York — We describe methods for projecting holographic optical traps whose potential energy wells are extended along specified curves, typically a straight line, and whose intensity profiles also can be tailored. This class of optical traps is useful for manipulating elongated nano-items, creating anisotropic potential energy landscapes, and in particular for investigating the interactions and dynamics of micro-particles in reduced dimensionality. This new class of extended optical traps is created by modulating the shape and the phase of a complex hologram, projected by a phase-only diffractive optical element. We demonstrate rapid characterization of extended traps' potential wells through digital video microscopy of trapped colloidal spheres, and use arrays of calibrated traps for efficient measurement and screening of colloidal interactions.

10:36AM G21.00014 Holographically Assembled Photonic Quasicrystals , YAEL ROICHMAN, DAVID G. GRIER, New York University — Recently, the photonic band structure of a centimeter-scale three-dimensional icosahedral quasicrystal was measured in the microwave region and shown to feature prominent photonic band gaps at the effective Brillouin zone boundary. We demonstrate that similar two- and three-dimensional quasicrystalline photonic structures can be assembled from micrometer-scale colloidal particles through dynamic holographic optical trapping. The resulting colloidal heterostructures feature lengthscales appropriate for photonic bandgap applications at visible wavelengths, and can include specifically engineered defects such as vacancies, active centers and waveguides.

#### 10:48AM G21.00015 The Intermediate Scattering Function in Fluorescence Correlation Spec-

**troscopy**, RODRIGO GUERRA, Harvard, BALLARD ANDREWS, PABITRA SEN, Schlumberger-Doll Research — We formulate the autocorrelation function for Fluorescence Correlation Spectroscopy (FCS)  $G_D(\tau)$  in reciprocal space in terms of the of the Intermediate Scattering Function ISF( $\vec{k}, t$ ) and the fourier transform of the Optical Response Function ORF( $\vec{k}$ ). In this way we may extend the use of FCS to processes that have been studied using NMR, DLS, and neutron scattering. This formalism is useful for the complicated propagators involved in confined systems and in the study of diffusion in cells: where diffusion is either restricted or permeation through membrane is important. Calculations in k-space produce approximate expressions for the ORF using cumulant expansions that are accurate for small wavevectors. This provides descriptions for longer timescales better suited for studying time-dependent diffusion  $ISF(\vec{k},t) \rightarrow exp[-tD(t)k^2]$  and provides a natural separation of contributions from system dynamics and from optical artifacts and aberrations. We will show an explicit derivation of a semi-analytical fit function for free diffusion based on standard electromagnetic analysis of a confocal optical apparatus. This fit function is then used to analyze a representative data set and has no free fit parameters other than the diffusion constant.

## Tuesday, March 14, 2006 8:00AM - 10:36AM – Session G34 DFD: Glassy Dynamics and Jamming Baltimore Convention Center 337

**8:00AM G34.00001 On the Lower Critical Dimension of the Edwards-Anderson Spin Glass**<sup>1</sup>, STEFAN BOETTCHER, Emory University, Physics Department — The Edwards-Anderson model of Spin Glasses is studied on dilute hyper-cubic lattices in dimensions d = 2, 3, ..., 7. Accurate predictions for the stiffness exponent  $y_d$  are obtained that describes low-energy excitations. Continuing  $y_d$  off the integers shows that its zero is located at d = 5/2 to within 0.1%, a prediction that is corroborated by other numerical and theoretical work. Related Publication: Phys. Rev. Lett. 95, 197205 (2005). Related Webpage: http://www.physics.emory.edu/faculty/boettcher/.

 $^{1}$ This work has been supported by grant 0312510 from the Division of Materials Research at the National Science Foundation and by the Emory University Research Council

8:12AM G34.00002 Direct measurement of the distinct part of van Hove correlation function  $G_d(r,t)$  in colloidal gels and glasses, YONGXIANG GAO, MARIA KILFOIL — Great effort has been put into understanding the mechanism and dynamics of glass formation, and progress has been made. It is now known that the cage effect causes the dynamical arrest, and thus the observed glass transition. This has been proven by direct observation by microscopy, by light scattering and rheology experiments of hard sphere systems near the glass transition, and by computer simulation. However, no real-space direct three dimensional measurements of large-length-scale dynamics have been done in glass samples. The distinct part of the van Hove correlation function  $G_d(r,t)$  provides direct access to the dynamics in glassy systems at all length scales. We use confocal microscopy to measure this function in both colloidal gels and glasses. Since both glass and gel formation are kinetic and not thermodynamic phenomena, we may expect that they share similarities. By looking at their dynamics, we may gain more insights into the unified jamming picture of liquid-to-disordered-solid transition.

8:24AM G34.00003 Fluctuations of Structure and Dynamics in an Aging Colloidal Glass<sup>1</sup>, GIANGUIDO C. CIANCI, ERIC R. WEEKS, Department of Physics, Emory University, Atlanta, GA 30322 USA — When a liquid is quenched to form a glass it becomes trapped in a non-equilibrium state. The non-ergodicity of the system is most clearly highlighted by the dependence of the glass' properties on the time elapsed since the quench. This phenomenon is known as aging. Dense colloidal suspensions have been shown to be a good model for the glassy state. We use fast laser scanning confocal microscopy to image sterically stabilized, micron-sized, PMMA spheres in three dimensions and track their positions over time with sub-pixel accuracy. While aging is most commonly detected by measuring the evolution of variables (such as the mean squared displacement or the intermediate scattering function) averaged over the entire system and over time these quantities cannot yield information about the detailed, structural changes that occur during aging. Confocal microscopy, on the other hand, allows us to intimately study the aging process with minimal or no averaging. We study the statistics of the fluctuations of geometrical and dynamical quantities over time as the sample ages. In particular, we find that the aging process is heterogeneous in time and space and compare the fluctuations of the aging process to intermittent, record induced dynamics models.

<sup>1</sup>Funding: NASA (NAG3-2728)

8:36AM G34.00004 Dynamic correlations and correlation length in the aging of a simple structural glass, AZITA PARSAEIAN, Department of Physics and Astronomy, Ohio University, HORACIO CASTILLO, Department of Physics and Astronomy, Ohio University — We present the results of a detailed molecular dynamics simulation of the spatial correlations of fluctuations in a simple binary Lennard-Jones glass former in the aging regime. We study the 4-point generalized density susceptibility  $\chi_4(t, t_w)$  and the dynamic correlation length  $\xi_4(t, t_w)$  associated with it, where  $t_w$  is the waiting time. We find that these data are consistent with the scalings  $\chi_4(t, t_w) = F(t_w)\chi_4^{0}(C(t, t_w))$  and  $\xi_4(t, t_w) = G(t_w)\xi_4^{0}(C(t, t_w))$ , where  $C(t, t_w)$  is the incoherent part of the intermediate scattering function. We also find that  $F(t_w)$  can be fit as a power of the waiting time, and  $G(t_w)$  can be fit as a logarithm of the waiting time. These differing time dependencies, plus the dramatically different behavior of the scaling functions  $\chi_4^0(C)$  and  $\xi_4^0(C)$  for small C lead to the conclusion that the time evolution of  $\chi_4(t, t_w)$  is not controlled by its associated dynamic correlation length  $\xi_4(t, t_w)$ .

#### 8:48AM G34.00005 Dynamic fluctuations of elastic lines in three-dimensional random enviro-

**ments**, SEBASTIAN BUSTINGORRY, Centro Atomico Bariloche, Argentina, LETICIA CUGLIANDOLO, LPTHE-Jussieu and LPT-ENS, Paris, DANIEL DOMINGUEZ, Centro Atomico Bariloche, Argentina — Elastic lines embedded in three-dimensional random environments present a low temperature glassy regime, with aging characterized by multiplicative scaling. We studied the scaling properties of the distribution functions of different dynamical observables: the roughness, the mean-squared-displacement and its associated response function. Following the multiplicative scaling hypothesis, we numerically show that the distribution functions depend only on the mean scaled value of the variables, and not on the different time scales involved. These results could be extended to the scaling of distribution functions in critical-like systems.

#### 9:00AM G34.00006 Microstructure of a polymer glass overaged by application of instantaneous

**shear strains**<sup>1</sup>, BELA JOOS, University of Ottawa, MATTHEW L. WALLACE, Université Louis Pasteur, Strasbourg — When applying a transient shear on jammed colloidal suspensions, Viassnoff and Lequeux (*Phys. Rev. Lett.* **89**, 065701 (2002)) observed both rejuvenation and overaging in the system, as the relaxation times are altered in a non- trivial way. Application of instantaneous, one-time shear deformations on a polymer glass by molecular dynamics simulations produces a similar behavior (M.L. Wallace and B. Joós, *Phys. Rev. Lett.*, in press). Two regimes are observed corresponding to elastic and plastic strains. Of particular interest are deformations in the plastic regime, above the yield strain ( $\epsilon > 0.1$ ), where the characteristic relaxation times  $\tau_{1/2}$  increase exponentially with  $\epsilon$ , after a long waiting time  $t_w$  following the deformation. We are in the process of understanding the nature of this state of the glass. There is a slight increase energy of the inherent structures  $\langle e_{IS} \rangle$ , in particular in the inter-chain component. The bond orientation of relaxation times. The average shifts to larger times, and the distribution broadens and resembles more a Gaussian. These properties suggest that, above the yield strain, the system becomes more homogeneous, and possibly less jammed.

<sup>1</sup>funded by NSERC (Canada)

9:12AM G34.00007 Observed Effects of Confinement on Colloidal Glasses<sup>1</sup>, CAROLYN NUGENT, HETAL PATEL, JOE SALDANA, ERIC R. WEEKS, Department of Physics, Emory University — We used a binary colloidal suspension to model glass molecules. By increasing the concentration of colloids, a glass transition is induced. Previous studies of colloidal suspensions show that as the glass transition is approached, colloids tend to move in groups of increasing size. In order to examine this phenomenon more closely, a colloidal suspension was confined between two parallel glass plates with a narrow gap of the order of a few colloid diameters in thickness. Confocal microscopy was used to observe the particles and follow their motion over time. We observed that motion in confined regions was much slower than motion in non-confined regions of the same sample. In addition, the motion perpendicular to the walls was slower than motion parallel to the walls. The arrangement of colloids into layers was also observed, which further influenced the motion.

<sup>1</sup>This project funded by NSF

9:24AM G34.00008 The effective temperature and the universal scaling behavior of aging colloidal glass system, PING WANG, CHAOMING SONG, HERNAN MAKSE, City College of New York, New York, NY 10031 — Mostly due to the enormous practical importance of glassy systems there has been a vast literature describing different theoretical frameworks for glasses, yet without a common theory applicable to the diverse range of systems undergoing a glass transition. Here we present experimental results on a simple glassy system pointing to a unifying view of out-of-equilibrium systems. We investigate correlation and response functions to external fields to monitor the aging of a colloidal glass composed of highly concentrated hard spherical particles suspended in an refraction index matched fluid for visualization. Our analysis reveals that even though the system is aging far from equilibrium, it behaves as it is equilibrated at a constant temperature, independent of the age. This temperature is larger than the bath, and can be rationalized by the cage dynamics in the system. Global and local fluctuations in the observables are also studied showing a common scaling behavior with the age of the system. While these results can be interpreted within the framework of unifying formulations of aging, the observed scaling forms of the correlation functions do not conform to the theoretical predictions.

9:36AM G34.00009 Aging of Johari-Goldstein Relaxation in Structural Glasses , HASAN YARDIMCI, ROBERT L. LEHENY, Department of Physics and Astronomy, Johns Hopkins University — Using frequency-dependent dielectric susceptibility measurements we characterize the aging in two supercooled liquids, sorbitol and xylitol, below their calorimetric glass transition temperatures,  $T_g$ . In addition to the alpha relaxation that tracks the structural dynamics, the susceptibilities of both liquids possess a secondary Johari-Goldstein relaxation at higher frequencies. Following a quench below  $T_g$ , the susceptibility slowly approaches equilibrium behavior. For both liquids, features of the Johari-Goldstein relaxation display a dependence on the time since the quench, or aging time, that is very similar to the age dependence of the alpha peak. However, one can not assign a single fictive temperature to both the alpha and Johari-Goldstein relaxations. For example, the peak frequency of the Johari-Goldstein relaxation remains constant during aging for sorbitol while it increases with age for xylitol, inconsistent with a decreasing fictive temperature. This behavior contrasts with that of the high frequency tail of the alpha peak whose shape and position track the aging of the main part of the peak.

9:48AM G34.00010 Glassy Dynamics in Suspensions of Non-Spherical Colloids , GALINA YATSENKO, KENNETH SCHWEIZER, University of Illinois, Urbana, IL 61801 — Glassy dynamics of isotropic fluids of hard symmetric dumbbells (diatomics), rods, cylinders and disks are studied using a simple form of mode coupling theory and its generalization to predict barriers and activated hopping transport. Orientational degrees of freedom dynamically enter in a pre-averaged manner, and structural correlations are quantified based on a center-of-mass version of the site-site Reference Interaction Site Model. A length-to-diameter (aspect) ratio serves as a principal parameter describing shape anisotropy. The ideal glass transition volume fraction of dumbbells is predicted to be a nonmonotonic function of aspect ratio. For continuous cylinders, ellipsoids and disks power law dependencies of glass transition volume fraction and localization length on aspect ratio are found in the highly anisotropic limit. The consequences of discotic liquid crystalline order for infinitely thin disks have also been studied. Multiple scaling behaviors with volume fraction and aspect ratio are predicted for the localization length, barrier height, elastic shear modulus and yield stress.

**10:00AM G34.00011 Microrheology of an aging colloidal glass**, S. JABBARI-FAROUJI, Univ. of Amsterdam, D. MIZUNO, M. ATAKHORRAMI, Free Univ. of Amsterdam, E. EISER, Univ. of Amsterdam, C. SCHMIDT, F. MACKINTOSH, Free Univ. of Amsterdam, G. WEGDAM, D. BONN, Univ. of Amsterdam — Laponite is a synthetic clay which after mixing with water, spontaneously evolves from an initially liquid and ergodic state to a non-ergodic glassy state that exhibits elastic behavior. We provide a direct experimental test of the Stokes-Einstein relation as a special case of the fluctuation-dissipation theorem (FDT) in this aging colloidal glass. The use of combined active and passive microrheology allows us to independently measure both the correlation and response functions in this non-equilibrium situation. Contrary to previous reports, we find no deviations from the FDT over several decades in frequency (1 Hz-10 kHz) and for all the observed aging times. Our measurements also demonstrate the applicability of fluctuation-based (passive) microrheology in a non-equilibrium glassy system. This method allows obtaining the viscoelastic properties over a very wide frequency range. Our striking observation is that there is a cross over in frequency behavior of complex shear modulus of system from single power law at early stages of aging to two power laws at later stages. This suggests the existence of two distinct viscoelastic contributions in the aging glass: (i) a high-frequency viscoelastic response in which the shear modulus increases rapidly with frequency; and (ii) a predominantly elastic (weakly frequency-dependent) response at lower frequencies, which becomes increasingly important as the system ages.

#### 10:12AM G34.00012 Activated Hopping and Dynamic Heterogeneity in Glassy Colloidal Sus-

**pensions**, ERICA SALTZMAN, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — A microscopic statistical dynamical theory of barriers and activated transport in dense colloidal suspensions has been developed by combining and extending methods of mode coupling, density functional and particle hopping theories. Quasi-analytic results for the mean relaxation time and ensemble-averaged transport coefficients agree well with experiment. However, a full determination of the dynamics requires numerical integration of the nonlinear overdamped stochastic equation of motion, i.e. Brownian dynamics simulation. This enables calculation of average quantities including the mean-square displacement, incoherent dynamic scattering function and alpha relaxation time, as well as trajectory-based quantities use as displacement and relaxation time distributions. Dynamic heterogeneity effects are explored by studying various decoupling factors, the non-gaussian parameter, the bimodality of the displacement distribution and the non-Fickian wavevector dependence of the structural relaxation time. Comparisons to mode-coupling theory, simulation and experimental results are performed.

#### 10:24AM G34.00013 Dependence of relaxation time on effective temperature in driven glasses<sup>1</sup>

THOMAS HAXTON, Physics Dept., Univ. of Pennsylvania, AJAY GOPINATHAN, Physics Dept., Univ. of California, Santa Barbara, ANDREA LIU, Physics Dept, Univ. of Pennsylvania — Relaxation times of a class of driven glassy systems are shown to depend on a well-defined effective temperature in much the same way that they depend on temperature in quiescent systems. Molecular dynamics simulations were run for two-dimensional systems of bi-disperse spheres interacting via soft repulsive pair potentials. At high density the systems undergo a glass transition as temperature is lowered. We study low-temperature systems driven by an imposed shear gradient in steady state at a fixed high density. Effective temperatures can be defined from fluctuation-dissipation relations by the long-time limit of the ratio of correlation to response. Throughout a range of bath temperatures and shear rates, relaxation times are found to depend on the relaxation time of the quiescent system as a function of T, using a scale factor that varies only weakly with the ratio  $T/T_{\rm eff}$ . This suggests that shear unjams the system because it gives rise to a  $T_{\rm eff}$  that is higher than the glass transition temperature.

<sup>1</sup>This work was supported by DOE grant DE-FG02-03ER46087.

## Tuesday, March 14, 2006 11:15AM - 2:15PM -

Session HŽÍ DFD: Focus Séssion: Microfluidic Physics I Baltimore Convention Center 318

11:15AM H21.00001 Experimental Studies of the Effects of Mixing on Reacting Systems<sup>1</sup>,

MATTHEW PAOLETTI, University of Maryland at College Park — Experimental studies of the effects of mixing on reacting systems are presented. The experiments can be divided into two classifications: (1) the effects of chaotic mixing on front propagation and (2) synchronization via superdiffusive mixing in an extended, fluid system. The front propagation studies are conducted in an oscillating vortex chain flow. The velocities of the propagating fronts are measured as a function of the frequency and amplitude of the external forcing. In the absence of mixing the Fisher-Kolmogorov result correctly predicts the front velocity; however these experiments show that this result is not extendable to chaotically mixed systems. Instead, the fronts are shown to mode-lock onto the external forcing, propagating an integer number of vortices in an integer number of drive periods. The flow used in the synchronization studies is an oscillating/drifting vortex chain, which may be used to produce both enhanced diffusion and superdiffusion. We show that the key to synchronization in an extended, fluid system is superdiffusive transport produced by Lévy flights, where tracers undergo rapid jumps between distant regions of the flow.

<sup>1</sup>Supported by NSF and Bucknell University Research Experience for Undergraduates

11:51AM H21.00002 Electrophoresis of Large DNA Molecules in Microcontractions , PATRICK DOYLE, GREG RANDALL, JU MIN KIM, MIT — The ability to controllably position and stretch large DNA molecules in a microfluidic format is important for gene mapping technologies such as Direct Linear Analysis (DLA). Current technologies developed for DLA use controlled hydrodynamic flows created in a microfluidic device. The downside to this approach is that the imposition of the no-slip condition at the channel walls generates vorticity which can lead to DNA chain tumbling and incomplete stretching. We have recently shown that electric field gradients can be readily generated in a microfluidic device and the resulting field is purely elongational. We present here single molecule studies of DNA molecules driven by an electric field through a microfabricated contraction. Analogous to the hydrodynamic deformation of DNA, we can define an electrophoretic Deborah number (De) for our problem. We will discuss the effectiveness of the device to fully stretch DNA as a function of De and compare to stretching achieved in hydrodynamic flows. A detailed analysis of molecular stretching and the role of a non-homogeneous electric field will be discussed.

12:03PM H21.00003 Measuring Streaming Current/Potential in Microchannel Arrays, ALI MAN-SOURI, AYDIN JAFARNEJAD, U of Alberta, DANIEL KWOK, U of Calgary, LARRY KOSTIUK, U of Alberta — Streaming current/potential measurements have been commonly used to estimate interfacial properties. This paper explores challenges in conducting these measurements in an array of parallel microchannels, which is akin to flow through porous media. The issue that arise with these arrays is that increasing the number of channels subsequently increases the total conductance across an array. In situations with a large number of channels this array conductance can become comparable to the conductance in the bulk fluid in the reservoirs where electrodes are placed. In these cases, current drawn through an external electrical circuit connecting the two reservoirs (i.e. streaming current) become highly dependent on the location, material and surface area of the electrodes. However, with fewer channels the relative magnitude of conductances can be made such that this externally measured current is independent of these parameters and more representative of the streaming current. Streaming potential measurement, since they do not involve external current flow, also do not show these dependencies. In this study variations in the electrode materials (bright platinum, platinized platinum, silver and stain steel), size of electrodes, placement of the electrodes and electrolyte concentration  $(10^{-3}M$ KCL,  $10^{-4}M$  KCL and 0 M KCL ) were used to affect the relative conductance in the system and to highlight these characteristics.

12:15PM H21.00004 Electrophoretic extraction of ions from a pressure-driven flow<sup>1</sup>, HAO LUO, BOYD EDWARDS, SCOTT MILLER, BRENT RESCHKE, AARON TIMPERMAN, WVU TEAM — Coupling pressure-driven and electrokinetically driven flow streams in microfluidics is a critical issue for developing multi-dimensional separations systems. A promising method of coupling these flows is to electrokinetically extract the charged components from the pressure driven flow stream while minimizing the hydrodynamic flow in the electrokinetically driven channel. To model this extraction process we calculate the fraction f of ions in a pressure-driven microchannel that are diverted electrophoretically to a perpendicular side channel. The channel cross sections are rectangular, with aspect ratio  $\gamma$ . In the main channel, we use truncations of an exact series solution to describe the laminar velocity profile of the aqueous solution. The aqueous solution in the side channel is stationary; individual ions move through this channel in response to a uniform applied electric field at an electrophoretic velocity that is proportional to this field. We calculate f as a function of  $\gamma$  and the ratio R between the flow rate in the main stream and that in the side stream. We find that f decreases with increasing R, as expected, and is nearly independent of  $\gamma$ . 12:27PM H21.00005 The effect of fluid density on the transport of particles in nanochannels, ZHIGANG LI, GERMAN DRAZER, Department of Chemical and Biomolecular Engineering, Johns Hopkins University — Understanding particle transport in nanochannels is crucial for the development of micro and nanofluidic devices. In this work, we investigate the effect of fluid number density on the transport of particles in nanochannels, by means of molecular dynamics simulations. Specifically, we examine the motion of a Lennard-Jones nanoparticle, under the action of a constant external force, in a Platinum nanochannel that contains a Lennard-Jones fluid. In the limiting case of a nanochannel free of fluid molecules the particle adsorbs to the surface of the nanochannel and moves at a very low velocity, due to dry friction with the wall. As the number density of the fluid increases the mobility of the nanoparticle is greatly enhanced, due to the formation of adsorbed fluid layers on the surface of both the nanochannel and the particle, which substantially reduce friction between the particle and the wall. Then, if the number density of the fluid is increased further the particle mobility drops, due to viscous drag. In fact, there is an optimal value at low fluid densities, at which the particle mobility can be significantly enhanced. We also examine the existence of a second peak at higher densities, when the fluid density is high enough to prevent the adsorption of the nanoparticles, and how these phenomena depend on the fluid-solid molecular interactions.

#### 12:39PM H21.00006 Molecular Dynamics simulations of polymers in Brownian ratchets.

MARTIN KENWARD, GARY W. SLATER, University of Ottawa — Brownian ratchets rely on a combination of thermal *noise* and an asymmetry in a system to induce directed transport of particles (e.g., pumping in ion channels). This is somewhat counter intuitive since thermal motion is often a detriment to transport mechanisms. In particular a Brownian ratchet can be used to manipulate polymers, for example in separation systems. We present a Molecular Dynamics study (with explicit hydrodynamic interactions) of short polymer chains in a fluid subjected to a periodic, asymmetric, saw-tooth potential (with zero net force) which is switched on and off for given time intervals,  $\tau_{on}$  and  $\tau_{off}$  repectively. We examine how variations of  $\tau_{on}$  and  $\tau_{off}$  affect the net migration of the polymer chains. We also examine how the width of the trapping potential and the degree of asymmetry affects the dynamics of the molecules.

12:51PM H21.00007 Self-Assembly of Paramagnetic Beads in Rotating Magnetic Fields<sup>1</sup>, ERIC KEAVENY, Division of Applied Mathematics, Brown University, MARTIN MAXEY, Division of Applied Mathematics, Brown University — Paramagnetic beads, about 1  $\mu$ m in diameter, suspended in a liquid will aggregate to form chains when an initially random dispersion is subject to a uniform, static magnetic field. In a rotating field, the chains deform and, depending on the rotation rate, form S-shaped chains or aggregate clusters. A correct determination of the final shape requires an accurate calculation of the interparticle forces. We developed new methods to efficiently and accurately calculate the far-field and near-field magnetic interactions. Hydrodynamic interactions are resolved through the force-coupling method. We study the dynamics of single chains and suspensions of beads in rotating fields using these models and compare results from our simulations with recent experiments by Melle et. al. (Phys. Rev. E **68**, 041503). At high rotations rates, the observed particle oscillations provide information on the particle properties affecting near-contact hydrodynamic forces.

<sup>1</sup>Supported by NSF award CTS-0326702

1:03PM H21.00008 Semiflexible magnetic filaments , ANDREJS CEBERS, Institute of Physics, Salaspils, LV-2169 — Extension of the Kirchhoff model of an elastic rod by taking into account the long-range magnetic interactions allows one to describe the semiflexible filaments with body couples. Their behaviour in some aspects is similar to the flagellas of different microorganisms driven by internal torques due to molecular motors. Basing on the model different new phenomena are described - buckling instability due to the action of body torques, selfpropulsion of the filament in an ac field, a periodic regime of the magnetic filament motion under the action of the shear flow and the field and others. Taking into account the thermal noise the crossover from  $t^{3/4}$  to  $t^{1/2}$  for the time dependence of the mean square displacement of the filament at magnetic field increase is predicted. The characteristics of semiflexible magnetic filaments can be studied by measuring their magnetic susceptibility in small ac magnetic field for which in the high- frequency range the scaling law  $\omega^{-3/4}$  is obtained. Application of these results for the study of the properties of magnetotactic bacteria is discussed.

1:15PM H21.00009 Using nanowires to perform in-vivo measurements of elastic and viscous properties of an anisotropic fluid , CHRIS SMITH, University of Western Ontario, COLIN DENNISTON, University of Western Ontario — The immersion of a small wire within an anisotropic fluid is studied using a lattice Boltzmann algorithm. A magnetic field is used to manipulate and rotate the wire. The field and the anisotropic fluid each impose a torque on the wire. Our simulations agree well with experiments on the dynamics of high aspect ratio wires within a liquid crystal. In addition, our simulations are able to extend the range of predictive measurements to low aspect ratio wires, more suitable for use in biological environments. We are able to predict elastic and viscous properties of the anisotropic fluid environment based on the torque response of the rotating wire.

1:27PM H21.00010 Experimental and theoretical study of mixing and transport due to the motion of a slender body sweeping out a cone.<sup>1</sup>, TERRY JO LEITERMAN, University of North Carolina at Chapel Hill, RICHARD M. MCLAUGHLIN, ROBERTO CAMASSA, UNC RTG FLUIDS GROUP TEAM — We have used singularity theory to construct an exact solution for the fluid motion induced by a spheriod spinning about its center sweeping out a double cone in a low Reynolds number flow. We have additionally used slender body theory to construct an asymptotic solution for a slender cylinder attached to a no-slip plane spinning about its base sweeping out an upright cone. These time-varying, three- dimensional hydrodynamic solutions have been used to benchmark micro-fluidic experiments which have immediate consequences to understanding transport and mixing in ciliated tissues. A similar macro-scale experiment that is absent of thermal flucutations has been designed which validates the theory.

#### $^1\mathrm{RTG}$ NSF DMS-0502266

1:39PM H21.00011 Field Effect Modulation of Ion Transport in Single Nanotubes, RONG FAN, PEIDONG YANG, Department of Chemistry, University of California at Berkeley — Field effect control in metal-oxide semiconductor field effect transistors (MOSFETs) has revolutionized how information is processed and stored, and created the modern digital age. Introducing field effect in fluidic systems would enable the manipulation of ionic and molecular species at a similar level and even logic operation. Due to strong Debye screening, field effect control in ionic solutions has to be occurring in nanoscale. Here we present the integration of chemically synthesized inorganic nanotubes into metal-oxide-solution field effect transistors (MOSoIFETs), and demonstrated a rapid field effect modulation of ionic conductance. Surface modification, functioning as doping in semiconductors, alters the nanofluidic transistors from p-type field effect transistors, to ambipolar FETs, and n-type field effect transistors. Ambipolar behavior is of special interests in this gapless transport system. Possion-Boltzmann model has been employed to extract two key physical parameters – zeta potential and surface charge density. Furthermore, transient study was conducted, leading to the first kinetic model of field effect in ionic solutions. Nanofluidic FETs would be the key elements in sub-femtoliter analytical techniques and the integration of large-scale nanofluidic circuits.

#### 1:51PM H21.00012 Performance based applications of the Ultrasound Contrast Agents in the

**bio-medical field**, PANKAJ JAIN, University of Delaware, KAUSIK SARKAR, University of Delaware — Ultrasound Contrast Agents are micron size bubbles encapsulated by nanometer-thick layer of surface active materials such as proteins and lipids. They are injected to patients to improve the quality of ultrasound images. They are also being used for drug delivery and arteriogenesis. We present results of *in-vitro* ultrasound investigation on two such contrast agents, Definity and Optison. We measure attenuation and scattering of ultrasound through emulsion of these agents. We investigate destruction of contrast agents and measure sub- and super-harmonic contents in their scattered response. Optison has a much lower threshold excitation level compared to Definity. Definity has a persistent sub-harmonic generation compared to Optison, for which the sub-harmonics go down above a certain pressure level. Both agents experiences transient bubble growth at lower excitation pressures due to increased permeability of the membrane to dissolved air outside. The results along with their implications on the applications such as drug delivery and imaging will be discussed.

2:03PM H21.00013 Tuning the orbital angular momentum in optical vortices , CHRISTIAN SCHMITZ, KAI UHRIG, JOACHIM SPATZ, JENNIFER CURTIS, Max-Planck-Institute for Metals Research, Dept. of New Materials and Biosystems, D-70569 Stuttgart, Germany — Optically-driven micromachines rely upon the precise definition of the intensity distribution and the angular momentum content of the controlling light fields. One such manipulation tool is the optical vortex (OV), which employs orbital angular momentum to spin particles around a ring of light. The orbital angular momentum of an OV is tuned by changing the helicity of its electric field's wavefronts or by tuning the input power. However, changing wavefront helicity has the undesirable effect of altering the vortex diameter. Thus, making complex patterns of OVs with fixed sizes but adjustable rotational frequencies is difficult. We introduce a new class of OVs with an additional independent tuning parameter to overcome these limitations. With these OVs, it is possible to smoothly increase particles' rotational frequency without changing the radius or power. We show that this tunability can be extended to groups of OVs with similar or different radii, allowing for complete flexibility to construct optical micromachines, or large arrays of OVs for parallel assays of biomolecules and cells.

#### Tuesday, March 14, 2006 2:30 PM - 5:18 PM $_-$

Session K21 DFD: Colloids V Baltimore Convention Center 318

2:30PM K21.00001 Giant Enhancement of Colloidal diffusion in a Corrugated Optical Vortex,

SANG-HYUK LEE, DAVID G. GRIER, Department of Physics and Center for Soft Matter Research New York University — We experimentally study thermally driven velocity fluctuations of a Brownian particle in a tilted washboard potential. Our system consists of a single fluid-borne colloidal sphere driven by a holographically projected superposition of optical vortices. A single optical vortex is a ring-like optical trap created by focusing a helical mode of laser light. Torque exerted by an optical vortex's orbital angular momentum flux drives a trapped colloidal particle around its circumference. Superposing two optical vortices with opposite helicities and different amplitudes creates a corrugated optical vortex with sinusoidal intensity variations around its circumference. The resulting tilted washboard potential admits both static trapped states and dynamic running states. Digital video microscopy measurements of the resulting particle trajectories reveal a hundred-fold enhancement of the effective self-diffusion coefficient near the static-to-running transition.

2:42PM K21.00002 Diffusion Limited Branched Polymers<sup>1</sup>, CARLOS MENDOZA, Instituto de Investigacion en Materiales, UNAM (MEXICO), GUILLERMO RAMIREZ-SANTIAGO, Instituto de Fisica, UNAM (MEXICO) — We introduce an algorithm to construct polymers with defined branching structure and whose morphology is determined by diffusion. We apply this procedure for the case of star-branched polymers and calculate their fractal dimension. We also carried out a finite size scaling analysis and determine the scaling properties of the radius of gyration. This procedure may be useful to construct large branched polymers near their relaxed configurations which in turn may help to determine equilibrium configurations of dilute solutions made of these polymers.

<sup>1</sup>Supported by DGAPA-UNAM IN110103 & CONACYT 43596-F

2:54PM K21.00003 A Constant Force Dielectrophoretic Cell, MARIA KILFOIL, VINCENT PELLETIER, ANDREW SCOTT, ALLAN HALDANE, McGill University — We fabricated an especially designed cell to study colloidal suspension under an isomotive dielectrophoresis force. Under such conditions, the effects of a uniaxial force on gel structure and crystallization can be studied with an absolute control on its magnitude. Since the force is horizontal by design, we can take advantage of the higher resolution on the horizontal axis to obtain more precise particle locations. Preliminary results are shown.

3:06PM K21.00004 Electric Double Layer Structures near Rough Surfaces: Molecular Dynamics Simulation, DAEJOONG KIM, ERIC DARVE, Stanford University — S. S. Dukhin in Surface and Colloid Science (1974) mentioned both the possibility of increase in zeta potential due to surface roughness and the possibility of decrease, depending on Debye length relative to surface roughness. In this work we report our results of molecular dynamic (MD) simulations on electric double layer structures near solid surfaces having roughness with the order of magnitude of Debye length. For computational simplicity only counter-ions are present. We computed static and dynamics properties including density profiles of water and ions, electrostatic potential distributions due to ions, polarization density profiles and self-diffusivities of water and ions. We also performed nonequilibrium MD to simulate electroosmotic flows. From electrostatic potential distributions and slip plane locations, we computed zeta potential and found that it decreases with surface roughness. It also showed a dependency on the spatial frequency of surface roughness. For comparison we used the Helmholtz-Smoluchowski relation and found the same trend. Currently we are studying pressure-driven flows, a computational counterpart to streaming current experiments. One of the purposes is to find more exact locations of slip planes by fitting to Poiseuille flow solutions. We are also simulating model systems with co-ions to investigate the possibility of charge inversion and other effects.

**3:18PM K21.00005 Heterogeneities in Two-Dimensional Pinned Liquids**, JING-XIAN LIN, T-12 and T-CNLS, Los Alamos National Laboratory; University of California, Riverside, CHARLES REICHHARDT, T-13 and T-CNLS, Los Alamos National Laboratory, ZOHAR NUSSINOV, T-11, Los Alamos National Laboratory, LEONID P. PRYADKO, University of California, Riverside, CYNTHIA J. OLSON REICHHARDT, T-12 and T-CNLS, Los Alamos National Laboratory — We introduce a model system in which the amount of heterogeneous motion in a liquid phase just above melting can be controlled directly. Using numerical simulations, we place a two-dimensional assembly of repulsively interacting colloids on a commensurate triangular substrate of pinning sites, and then randomly deactivate a fraction  $n_p$  of the pinning sites. Heterogeneous motion is induced when the unpinned colloids, and this heterogeneity can be controlled by changing the fraction of active pinning sites. The melting transition occurs in a single step for  $n_p = 0$  or 1, and is considerably broadened for partially pinned samples. We measure the noise fluctuations of the dislocation density as a function of time and find a maximum noise power when  $n_p = 0.5$ . Signatures of a two step melting process appear for up to 3/4 of the pinning sites removed. We also correlate the regions of high mobility with regions of high dislocation density, and analyze the heterogeneity using the Van Hove correlation.

3:30PM K21.00006 Computation of Super-Hydrophobic States and Stability<sup>1</sup>, YONGKANG CHEN. Portland State University, DANNY BOLLEDDULA, RYAN JENSON, MARK WEISLOGEL — Super-hydrophobic fluid phenomena have been the focus of an increasing number of research investigations over the past decade. Perhaps the greatest achievements recently have come by way of the highly controlled surfaces that can be produced using any one of a number of rapidly expanding surface microfabrication techniques. In this work we present a numerical approach to systematically probe both the states and stability of certain (super- or ultra-) hydrophobic surfaces as they depend on surface porosity, specific surface feature size and geometry, and fluid properties such as 'equilibrium' contact angle and surface tension. Drop stability in terms of critical roll-off angles, advancing and receding contact angles (hysteresis), Bond number, and effective contact angle is computed and used as a measure of 'super-hydrophobicity.' Both Wenzel and Cassie hydrophobic states are analyzed by the numerical method.

<sup>1</sup>Support for this research provide by the National Science Foundation (CTS-0521890)

3:42PM K21.00007 Design of Porous Wick Structures: Steady Flows<sup>1</sup>, Mark Weislogel, Ryan Jenson, YONGKANG CHEN, LAWRENCE MELVIN III — Methods of analysis developed for capillary flows in large complex containers for spacecraft are applied to microscale networks of interconnected repeat units to develop design methodologies to compute optimal geometries for high performance microporous materials and structures on Earth. The fundamental transport mechanism in the media is the interior corner geometry. The specific objectives of the research focus on the optimization of high performance wick structures employed in advanced two-phase passive cooling systems for microelectronic thermal control. The analysis employs the governing transport equations in a cell-by-cell approach to compute optimal pore structures in the low saturation limit where the media may be effectively modeled as a nodal network of interconnected interior corners and solved by matrix methods. The 'all analytic' method under development does not employ empirically determined constants or highly varying numerical coefficients as other pore-scale investigations. Example pore geometries solved to date for steady flows clearly identify the origins of the manifold improvements possible in select porous structures. Applications for such methods are also helpful to improving transport processes in porous media such as fabrics and membranes.

<sup>1</sup>Support for this work provide by the National Science Foundation (CTS-0521890)

3:54PM K21.00008 Capillary waves at the water liquid-vapor interface, Ahmed E. Ismail, Gary S. GREST, MARK J. STEVENS, Sandia National Laboratories — Evidence for capillary waves at the liquid-vapor interface of water is presented from molecular dynamics simulations. The total interfacial width includes a correction term which depends logarithmically on the length  $L_{\parallel}$  of the simulation cell parallel to the interface, and which is inversely proportional to the surface tension  $\gamma_{cw}$ . Comparison of  $\gamma_{cw}$  for system sizes up to  $10^5$  molecules to  $\gamma_p$ , obtained from the difference between the pressure parallel and the pressure perpendicular to the interface, yields adequate agreement only if one fits the interfacial profile to an error function and not to a hyperbolic tangent, as often assumed. Results for  $\gamma$  for a number of atomistic three-site (SPC/E, TIP3P, TIP3P-CHARMM, and TIP3P-Ew) and four-site (TIP4P and TIP4P-Ew) non-polarizable water models are compared to experiment for temperatures from 300 K to 500 K, and for a variety of interaction cutoffs and reciprocal-space mesh refinements. Our results show that the SPC/E model is more accurate than the other available three-site models, while the original TIP3P model is closer to experimental data than its more recent parameterizations.

4:06PM K21.00009 Self-assembly of Colloid-Polymer Mixtures Confined by Soft Walls, YU-QIANG MA, National Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, China — We discuss how to control self-assembled ordering structures in colloid-polymer systems confined by soft walls, and find that with varying the colloidal concentration, the colloidal self- assembly undergoes a series of symmetry-changing transitions, due to the competition between the elastic entropy effect of soft walls and steric packing effect of colloids.

#### 4:18PM K21.00010 Rheological response of emulsions of drops immersed in electric fields.

ARTURO FERNANDEZ, The Catholic University of America – Direct numerical simulation is used to examine the temporal response of an emulsion of drops immersed in an electric field. When a drop is immersed in a suspending fluid of different electrical properties, and an electric field is applied, surface electric charges accumulate on the boundary between drop and suspending fluid. These charges, coupled with an electric field, lead to the appearance of electric stresses at the interface between the fluids. When an emulsion is immersed between two plates moving at different velocities, the microstructure and rheological properties depend on the competition between electric and hydrodynamical forces. We present a study of these phenomena for DC and AC electric fields. The effect on microstructure is quantified by the PDF, and on rheological properties by effective viscosity and normal stress difference. The numerical simulations show that fluid shear, electrical properties of both fluids, frequency for an AC electric field, and intensity are the main parameters governing the response of the system.

4:30PM K21.00011 Applications of Quartz Tuning Forks to Liquid Property Measurements , JAMES BENNETT, LEONID MATSIEV, OLEG KOLOSOV, Symyx Technologies — Sensor technology for fluid samples often measures a single physical parameter per sensor and for many applications this is sufficient. In some cases however, characterization of the state or condition of a fluid can be improved through the simultaneous measurement of multiple physical parameters. We will discuss our work in the application of flexural mechanical resonators such as quartz tuning forks to the characterization of fluids. We have previously shown that if a tuning fork resonator is immersed in a fluid, the changes in resonator response can be used to determine physical properties of the fluid. We will describe the development of a measurement system based on a tuning fork resonator, the associated electronics and analysis software. This system can provide simultaneous measurement of liquid properties such as viscosity, density, dielectric constant and ac conductivity. We have applied the tuning fork sensor to the characterization of fluids over a range of temperatures and conditions. Simultaneous measurement of viscosity, density and dielectric constant can provide information about the state or condition of the fluid. For example, for motor oils, clear differences in the measured parameters are observed between fresh and used oils and may be correlated to the oil condition.

#### 4:42PM K21.00012 Phase Segregation and Patterning in Two Dimensional Systems: Competi-

tion Between Van der Waals and Electrostatic interactions, SHARON LOVERDE, Department of Materials Science and Engineering, Northwestern University, FRANCISCO SOLIS, Department of Biophysics, Arizona State University, MONICA OLVERA DE LA CRUZ, Department of Materials Science and Engineering, Northwestern University — The formation of heterogeneities on surfaces, such as microdomains found in synthetic and natural lipid membranes, has not yet been yet fully explored from a theoretical point of view. It has been proposed, for example, that lipid rafts arise in membranes due to lipid-lipid and/or lipid-protein interactions. We consider a coarse-grained model of a mixture of charged lipids interacting within a monolayer. We analyze this model both analytically and with molecular dynamics simulations, and find a rich phase diagram. The complex phase behavior is generated by the competition between the short range van der Waals interactions and long range electrostatic interactions. In particular, we observe phase coexistence between an "ionic gas" phase with a dense patterned solid phase. We have examined the phase diagram of the system as a function of net charge density and charge asymmetry.

4:54PM K21.00013 Binary Lennard-Jones Fluids: A Look Through Time Series Analysis<sup>1</sup>, THEODOROS KARAKASIDIS, ATHANASIOS FRAGKOU, ANTONIOS LIAKOPOULOS, Hydromechanics Laboratory, School of Engineering, University of Thessaly, 38334 Volos, Greece — In this paper we discuss the dynamical behavior of a binary Lennard-Jones fluid simulated at the atomic scale using Molecular Dynamics. The system was simulated at several fluid states as a function of system density and temperature and its instantaneous temperature was recorded. We report preliminary results on time-series analyses of the instantaneous system temperature as well as of the temperature of its two constituents. In this course we employ both linear (autocorrelation function and power spectrum) and non-linear tools (average mutual information and correlation dimension). It turns out that the time series present a complex  $1/f^{\alpha}$  behavior. The dependence of the regimes on the physical state of the system is discussed.

<sup>1</sup>Acknowledgements: This research has been partially supported by the program "PYTHAGORAS-EPEA K II" jointly funded by the European Community and the Greek Ministry of Education.

5:06PM K21.00014 2D Lennard-Jones as complex liquid , ALEXANDER PATASHINSKI, Northwestern University, RAFAL ORLIK, ANTONI MITUS, Polytechnic University, Wroclaw, Poland, MARK RATNER, Northwestern University — The high viscosity, large relaxation times, and other signature features of complex liquids are associated with substantial local order and long-living significant liquid structures in these liquids. In 3D Lennard-Jones liquid appears locally ordered: about half of the atoms are, at any time, in recognizable hexagonal cages. We present results of a study of the statistics and dynamics of local order in 7-atom clusters in 2D Lennard-Jones-based system. The study includes states along a supercritical isotherm in the range of densities where the system changes from disordered liquid to ordered solid state.

## Wednesday, March 15, 2006 8:00AM - 11:00AM -

Session N8 DFD: Granular Flows Baltimore Convention Center 314

8:00AM N8.00001 Assessing a Continuum Description of Wide Shear Zones in Slow Granular Flow by Discrete Element Simulations, JEREMY B. LECHMAN, GARY S. GREST, Sandia National Laboratories\*, MARTIN DEPKEN, Instituut-Lorentz for Theoretical Physics, MARTIN VAN HECKE, Kamerlingh Onnes Lab — While the rheology of rapid granular flows is becoming well established, slow, dense flows are not well characterized in part because the strain localization (i.e., shear bands) they often exhibit is not easily amenable to continuum descriptions. Recently, a novel experimental system (split-bottom Couette Cell) was developed with promising potential to give new insight into these flows due to its wide, smooth shear zones (Fenistein et al. PRL 92, 94301). Subsequent experimental and numerical studies have lead to a good understanding of the nature of the flow in this device, which has lead Depken et al. (cond-mat/0510524) to propose a set of testable constitutive relations between the internal stresses and flow field. In particular, they suggest that the bulk, effective friction coefficient between sliding layers of particles is not constant, but has a subtle dependence on the orientation of the layers with respect to the bulk force. Here we present large-scale Discrete Element Simulations to analyze the bulk flow in both circular, above and below the critical height, and linear, where no critical height for slip at the base is found, split-bottom geometries. We check the proposed form of the stress tensor and assess the validity of the claim that the effective friction coefficient depends on the shape of th

8:12AM N8.00002 Dynamical heterogeneities in dense granular flow: timescales and largescale particle rearrangements, ALLISON FERGUSON, BULBUL CHAKRABORTY, Brandeis University — Recent interest in understanding the dynamical arrest leading to a fluid  $\rightarrow$  solid transition in both thermal and athermal systems has led to questions about the nature of these jamming transitions (PRL 86, 111 (2001), Nature 411, 772 (2001)). It is believed that these jamming transitions are dependent on the influence of extended structures on the dynamics of the system (Science 287, 627 (2000)). Simulations of steady-state gravity-driven flows of inelastically colliding hard disks show the formation of large-scale linear chains of particles with a high collision frequency even at flow velocities well above the jamming transition (EPL 66, 277 (2004)). These chains can be shown to carry much of the collisional stress in the system due to a dynamical correlation that develops between the momentum transfer and time between collisions in these "frequently-colliding" particles. While measurements of slowly decaying stress correlations yield an average lifetime for these structures which scales inversely with the flow velocity (cond-mat/0505496), distributions of time scales associated with the stress chains may provide more information about their effect on the dynamics of the flowing granular medium. These distributions may be obtained by considering time scales related to large-scale rearrangements of neighbouring particles in analogy with measurements done on supercooled fluids.

8:24AM N8.00003 Dense granular flows down an inclined plane, ROBERT ECKE, TAMAS BORZSONYI<sup>1</sup>, Los Alamos National Laboratory — Granular flow on a rough inclined plane is an important model system in which to study the basic rules of the dynamics of granular materials. Despite intensive study, many features of such flows are still incompletely understood. For uniformly flowing layers at relatively shallow inclination, we consider experimentally the the basic flow rheology of the granular media and propose new scalings to collapse our data for glass beads and rough sand as a function of inclination angle and particle diameter. At steep inclinations above some angle  $\theta_s$  ( $\tan \theta_s / \tan \theta_r \approx 1.3 - 1.5$ , where  $\theta_r$  stands for the angle of repose) for flowing grains, numerics and theory predict that the surface roughness is inadequate to dissipate energy gained in the gravitational field, and the flow should continue to accelerate. We report on our experimental results on the properties of granular flows on a steeply inclined plane and define the domains of steady flows. We also discuss the instabilities of such flows leading to spatial patterns.

<sup>1</sup>Currently at Hungarian Academy of Sciences, Budapest, Hungary

8:36AM N8.00004 Transverse Instability of Avalanches in Granular Flows down Incline<sup>1</sup>, IGOR ARANSON, Argonne National Laboratory, FLORENT MALLOGGI, ERIC CLEMENT, ESPCI, France — Avalanche experiments on an erodible substrate are treated in the framework of "partial fluidization" model of dense granular flows. The model identifies a family of propagating soliton-like avalanches with shape and velocity controlled by the inclination angle and the depth of substrate. At high inclination angles the solitons display a transverse instability, followed by coarsening and fingering similar to recent experimental observation. A primary cause for the transverse instability is directly related to the dependence of soliton velocity on the granular mass trapped in the avalanche.

<sup>1</sup>This research was supported by US DOE, contract #W-31-109-ENG-38

8:48AM N8.00005 Swirling in a Vibrated Monolayer of Rods, VIJAY NARAYAN, SRIRAM RAMASWAMY, Indian Institute of Science, Bangalore, NARAYANAN MENON, U. of Massachusetts, Amherst — We report observations of the spatiotemporal behaviour of a vertically vibrated horizontal monolayer of copper rods (aspect ratio  $\approx$  5) etched to a rolling-pin-like shape. The spatial organization of the rods resembles a highly-defected nematic state with large, coherently moving swirls. We measure spatiotemporal correlations of the single-particle and collective velocities, and study the structure and dynamics of the system as a function of density and vibration amplitude. We analyze the observed patterns in the light of theories<sup>1</sup> of orientational ordering, dynamics, and topological defects in systems of driven particles. We make comparisons to related but different experiments<sup>2</sup>, as well as to our earlier measurements<sup>3</sup> on similar particles with higher aspect ratio.

<sup>1</sup> J. Toner, Y. Tu and S. Ramaswamy, Ann. Phys. 318 (2005) 170.

 $^2$  D.L. Blair, T. Neicu, and A. Kudrolli, Phys. Rev. E 67, 031303 (2003).

<sup>3</sup> V. Narayan, N. Menon and S. Ramaswamy, J. Stat. Mech. (2005) in press; cond-mat/0510082.

#### 9:00AM N8.00006 Simple Power Law for Transport Ratio with Bimodal Distribution of Coarse

Sediment, CHRISTOPHER THAXTON, Appalachian State University, JOSEPH CALANTONI, Naval Research Laboratory — Using a discrete particle model, we have simulated sheet flow transport of coarse bimodal sediment distributions in the bottom boundary layer over a range of oscillatory waves and steady currents. The ratio of large grain to small grain diameter was varied as 5:4, 3:2, and 2:1. For each bimodal distribution, the mass ratio  $M_L/M_S$  ( $M_L$  and  $M_S$  are the masses of large and small grains respectively – the total mass was fixed for all runs) was varied from 1/9 up to 9/1. We find that, independent of wave and current forcing for the range of conditions considered, the ratio of large to small grain time-average transport rate obeys the power law  $Q_L/Q_S = C(M_L/M_S)^k$ , where  $Q_L$  and  $Q_S$  are the time-average transport rates of the large grains and small grains respectively and C and k are regression constants. A linear regression in log space (including 81 different simulations per diameter ratio) suggests that  $k \approx D_L/D_S$  with R<sup>2</sup> >0.9. The robust nature of the results suggests that the new power law may have a broad range of applications for shear flows of bimodal granular mixtures.

#### 9:12AM N8.00007 Large scale surface flow generation in driven suspensions of magnetic mi-

**croparticles.**, MAXIM BELKIN, ALEXEY SNEZHKO, IGOR ARANSON, Materials Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne IL 60439 — Nontrivially ordered dynamic self-assembled snake-like structures are formed in an ensemble of magnetic microparticles suspended over a fluid surface and energized by an external alternating magnetic field. These self-assembled multi-segment structures emerge as a result of the collective interaction between the particles oscillations induced by an external magnetic field and the standing waves on the surface of fluid. Surprising large-scale vortex flows are generated by these snake-like structures. The flows can be as fast as 2 cm/sec and strongly depend on the driving magnetic field parameters. We report on systematical experimental study of the vortex flow properties and generation mechanisms.

9:24AM N8.00008 Green-Kubo expressions for transport coefficients of a granular fluid. , APARNA BASKARAN, JAMES DUFTY, Department of Physics, University of Florida — A formal derivation of linear hydrodynamics for a granular fluid is given. The linear response to small spatial perturbations of the homogeneous state is studied in detail using methods of nonequilibrium statistical mechanics. A transport matrix for macroscopic excitations in the fluid is defined in terms of the response functions. An expansion in the wavevector to second order allows identification of all phenomenological susceptibilities and transport coefficients through Navier - Stokes order [1]. The transport coefficients in this representation are the generalization of Helfand and Green-Kubo relations to granular fluids. The analysis applies to a wide range of collision rules. Several differences from the corresponding expressions in the elastic limit are noted. Then, the particular case of inelastic hard spheres is considered and some approximate analytical evaluations illustrated. [1] A preliminary report of these results can be found in J. W. Dufty, A. Baskaran and J. J. Brey cond-matt/0507609

#### 9:36AM N8.00009 Dynamics angle and surface flow properties of wet and cohesive granular

**matter**, QING XU, ARSHAD KUDROLLI, Physics Dept., Clark University — We will discuss an experimental study of the flow of grains mixed with a small amount of liquid using a horizontally rotated drum apparatus, extending on our previous work on the maximum angle of stability of wet granular materials [1]. We focus on the continuous avalanching regime observed at high rotation rates, and examine the shape of the granular surface and depth of flow with imaging techniques as a function of amount, viscosity and surface tension of the liquid. Glass beads with 1mm diameter, and a drum with a diameter 295 mm and a width of 145mm is used to minimize the effect of the boundary. We find that the shape of the surface may be approximated by two linear segments in the upper and lower halves. The slope of the upper segment corresponding to the dynamical angle of repose  $\theta_d$  is observed to initially increase with rotation rate and volume fraction of liquid as expected, while the lower segment has an approximately constant slope. Interestingly,  $\theta_d$  is observed to peak before decreasing to an approximately constant value as the volume fraction is increased. The rate of increase of  $\theta_d$  is observed to decrease with rotation rate and viscosity. The role of the time scale over which wet grains shear past each other and the time over which grains actually come into contact due to lubrication forces on the observed change in scaling will be discussed.

[1]: S. Nowak, A. Samadani, and A. Kudrolli, Nature Physics 1, 50 (2005).

#### 9:48AM N8.00010 Characterizing the banded state of granular material in a rotating drum.<sup>1</sup>,

MICHAEL NEWEY, University of Maryland, KENNETH DESMOND, Rochester Institute of Technology, WOLFGANG LOSERT, University of Maryland — Why do particles of different size segregate axially in a horizontal rotating tumbler? We aim to understand the microscopic mechanisms for axial segregation through direct measurements of the motion of individual particles. Imaging the surface of the flowing layer, we extract flow angles, velocities, drift and diffusion for different particle types and mixtures of particles. Surprisingly, the direction of surface drift and steepest flow angle do not coincide and that surface drift cannot explain the axial segregation in our mixtures. On the other hand, particles in small particle bands flow significantly faster then particles in large particle bands, and this can be observed before visible band formation. We discuss the possible role of velocity differences in the axial segregation process. We characterize the fluidity of the flowing layer from its response to gentle sideways forcing.

<sup>1</sup>Supported by NASA Grant NAG-32736

#### 10:00AM N8.00011 Mechanisms in size segregation of binary granular mixtures, stephan ulrich,

University of Göttingen, JENNIFER KREFT, MATTHIAS SCHRÖTER, JACK SWIFT, HARRY SWINNEY, Center for Nonlinear Dynamics, University of Texas at Austin — Shaking of a mixture of large and small particles can lead to segregation. One distinguishes between the Brazil-nut effect (large particles go to the top) and its opposite, the reverse Brazil-nut effect. In this talk, experiments of vertically shaken binary mixtures are presented. Using image analysis, the number of large particles visible at the top and bottom of the granulate are counted to determine the state of segregation. By complementing these results with molecular dynamics simulations, we are able to identify different segregation mechanisms discussed in recent theoretical approaches: a geometrical mechanism called void filling, transport of particles in sidewall-driven convection rolls, and thermal diffusion, a mechanism predicted by kinetic theory.

10:12AM N8.00012 Upward penetration through a granular medium , D. COSTANTINO, T.J. SHEIDEMAN-TEL, M.B. STONE, J. COLE, C. CONGER, K. KLEIN, M. LOHR, W. MCCONVILLE, Z. MODIG, P. SCHIFFER, Penn State University — We measure the force needed to push a flat plunger upwards through a granular medium. The plunger begins flush with the base of the grains' container, and we focus upon the force necessary to initiate motion. The data show that this break-out force increases monotonically with plunger diameter and pile height as expected. In contrast to previous measurements of the force needed for vertical penetration from above and of the horizontal drag force, this break-out force has a strong dependence on head dispersive. Descente purchad by NASA event NACS 2000 and the NESE DEL measurements of the strong the NASA event NACS and the NESE DEL measurements of the strong the NASA event NACS and the NESE DEL measurements of the strong the NASA event NACS and the NESE DEL measurements of the strong the NASA event NACS and the NESE DEL measurements of the strong the stro dependence on bead diameter. Research supported by NASA grant NAG3-2384 and the NSF REU program.

10:24AM N8.00013 Correlation in granular shear flows, GREGG LOIS, University of California, Santa Barbara, JEAN CARLSON, University of California, Santa Barbara — We investigate the effects of long-range correlation in simulations of sheared granular materials and develop theories to model force propagation in the dense regime. Measurements of spatial force correlations determine the size of force networks that emerge as the density is increased. The magnitude of the correlation length separates the dilute regime, where kinetic theory holds, from a dense regime where its assumptions break down. In the dense regime we introduce theories that successfully predict constitutive relations for the stress tensor, using geometrical properties of the force networks. Additionally, we observe that the behavior of the contact force distribution at small forces is highly dependent on the size of the force networks

 $10:36AM\ N8.00014\ Shear\ reversal\ in\ granular\ flows\ ,\ {\sf MASAHIRO\ TOIYA\ ,\ University\ of\ Maryland\ ,\ WOLFGANG\ LOSERT\ ,\ University\ of\ Maryland\ -\ The\ reversal\ of\ the\ shear\ direction\ in\ flow\ of\ monodisperse\ and\ bidisperse\ granular\ matter\ in\ a\ shear\ cell\ of\ Taylor-Couette\ type\ is$ characterized experimentally. By changing the boundary conditions we tune the location and width of the shear band in steady state flow. When the shear direction is reversed, the system compacts over a characteristic length of half a particle diameter, and shear forces reach a steady state over a chacteristic length of 1-3 particle diameter. A linear strain is found at the onset of shear reversal before a steady state shear band develops. We associate this extra strain during shear reversal with the displacement needed to jam particles in regions away from the shearband. We find that the strain decreases with increasing particle size for a fixed system size. We also find radial components in average particle velocities at the top surface, suggesting a convection current in the bulk.

10:48AM N8.00015 Flux from a vibrated granular medium , KE CHEN, MATTHEW STONE<sup>1</sup>, RACHEL BARRY, MATTHEW LOHR, WILLIAM MCCONVILLE, Dept. of Physics and Materials Research Inst., Penn State University, KIT KLEIN, Dept. of Computer Engr., Penn State University, BEN-LI SHEU, Dept. of Physics and Materials Research Inst., Penn State University, ANDREW MORSS<sup>2</sup>, Dept. of Physics and Materials Research Inst., Penn State University, THOMAS SCHEIDEMANTEL, PETER SCHIFFER, Dept. of Physics and Materials Research Inst., Penn State University — We have studied vertically vibrated granular media by measuring the flux through a hole in the container's bottom surface. We find that when fully fluidized, the flux is controlled by the peak velocity of the vibration,  $v_{max}$ , i.e., the flux is nearly independent of the frequency and acceleration amplitude for a given value of  $v_{max}$ . The flux decreases with increasing peak velocity and then becomes constant for the largest values of  $v_{max}$ . We demonstrate that the data at low peak velocity can be quantitatively described by a hydrodynamic model. By contrast, the nearly constant flux at larger peak velocity signals a crossover to a state in which the granular density near the bottom is insensitive to the energy input to the system. This research was supported by the NASA through grant NAG3-2384 and the NSF REU program through grant DMR 0305238.

<sup>1</sup>Currently at Condensed Matter Sciences Division, Oak Ridge Natl. Lab <sup>2</sup>Currently at Dept. of Physics, Ohio State University

#### Wednesday, March 15, 2006 8:00AM - 10:48AM -Session N21 DFD: Microfluidic Physics II Baltimore Convention Center 318

8:00AM N21.00001 Microfluidics with Gel Emulsions, CRAIG PRIEST, ENKHTUUL SURENJAV, STEPHAN HER-MINGHAUS, RALF SEEMANN, Max-Planck-Institute for Dynamics and Self-Organization — Microfluidic processing is usually achieved using single phase liquids. Instead, we use monodisperse emulsions to compartment liquids within microchannel geometries. At low continuous phase volume fractions, droplets self-organize to form well-defined arrangements, analogous to foam. While it is well-known that confined geometries can induce rearrangement of foam com-partments at the millimeter-scale, similar dynamics are also expected for gel emulsions. We have studied online generation, organization and manipulation of gel emulsions using a variety of microchannel geometries. "Passive" reorganization, based on fixed channel geometries, can be supplemented by "active" manipulation by incorporating a ferrofluid phase. A ferromagnetic phase facilitates reorganization of liquid compartments on demand using an electromagnetic private coalescence between adjacent compartments within a gel emulsion can be induced using electrical potential. Microfluidics using gel emulsions trigger. Moreover, coalescence between adjacent compartments within a gel emulsion can be induced using electrical potential. Microfluidics using gel emulsions will be well-suited for combinatorial chemistry, DNA sequencing, drug screening and protein crystallizations.

#### 8:12AM N21.00002 In-situ Generation of Focal Conic Defects in Flow of Smectic-A Liquid

Crvstals in Microchannels<sup>1</sup>, SHAHAB SHOJAEI-ZADEH, SHELLEY ANNA<sup>2</sup>, Carnegie Mellon University — The response of ordered phases of layered liquids such as smectic-A liquid crystals to flow is often dominated not by the direct coupling of flow to molecular degrees of freedom, but by the driven motion of defects in these systems. This is because flow generates instabilities in these systems that lead to the formation of defects. Most attention to date focuses on the global viscoelastic behavior and shear alignment of layered liquids, while little work has been done to understand defect motion and defect/flow interaction in these systems. Here we introduce a new approach, which enables simultaneous generation and observation of focal conic defects in pressure-driven flow of smectic-A liquid crystals. We observe that introducing a sudden change in the cross-sectional area of a microchannel via a small obstacle leads to the formation of a steady stream of defects. Generated defects move along the microchannel and interact with each other and with the flow itself. We measure the pressure drop and defect velocity and relate these to observed defect size and microchannel geometry. These results provide a novel way of probing nonlinear behavior of layered fluids under flow.

<sup>1</sup>This research is supported by NSF Grant CTS-0527909.  $^{2}$ Department of Mechanical Engineering

8:24AM N21.00003 Folding and swirling of viscous threads in microfluidics, thomas cubaud, thomas G. MASON, UCLA, Chemistry and Biochemistry Dept. — We study miscible multiphase flows with large viscosity contrast in microchannels. We investigate the folding instability of a viscous thread surrounded by a less viscous liquid that flow into a diverging microchannel. In this situation, extensional viscous stresses cause the thread to bend and fold rather than dilating in order to minimize dissipation. We show that diffusive mixing at the boundary of the thread can significantly modify the folding flow morphologies. We relate the folding frequency to the characteristic shear rate. We also examine the hydrodynamic coupling between multiple threads and the threads' rupturing into arrays of viscous swirls, reminiscent of the Kelvin-Helmholtz instability.

#### 8:36AM N21.00004 Observations of Tipstreaming and Thread Formation in a Microfluidic

Flow Focusing Device , SHELLEY ANNA, Carnegie Mellon University, HANS MAYER, Department of Mechanical Engineering, Carnegie Mellon University — We present a novel method of generating sub-micron scale droplets in a microfluidic device. In particular we utilize the interaction of fluid motion and surfactant transport during the tipstreaming mode of droplet formation, which is achieved using a flow focusing microfluidic design. Tipstreaming is a mode of drop breakup in which daughter droplets, usually orders of magnitude smaller than the parent drops, are ejected from the pointed tips of parent droplets or bubbles. An attractive characteristic of tipstreaming is that droplets produced are not limited by the device feature size. In this work we observe that tipstreaming occurs within a specific range of capillary number (Ca  $\sim 0.1$  to 1, consistent with literature values for tipstreaming), flow rate ratio, and surfactant concentration, and that tipstreaming is preceded by the formation of thin threads that follow the pinchoff of larger droplets. We measure the thread diameter and length as a function of dimensionless parameters and discuss our results with respect to surfactant diffusion and kinetic timescales relative to flow timescales.

8:48AM N21.00005 Drops and Jets in two Phase Coaxial Flows, ANDREW UTADA, ALBERTO FERNANDEZ-NIEVES, DAVID WEITZ, Harvard University — We discuss the transition from dripping to jetting from a nozzle in a coaxially flowing fluid. The fact that the outer fluid is viscous and moving affects the transition from dripping to jetting as well jet shape and drop formation mechanism. We relate the physics of drop formation to a recently reported microcapillary device (1,2) that generates monodisperse double emulsions. (1) A. S. Utada, E. Lorenceau, D. R. Link, P. Kaplan, H. A. Stone, D. A. Weitz, Science 308, 537 (2005) (2) E. Lorenceau, A. S. Utada, D. R. Link, G. Cristobal, M. Joanicot, D. A. Weitz, Langmuir in press, (2005).

#### 9:00AM N21.00006 Geometrically controlled jet-like instabilities in microfluidic two-phase

**flows**, KATHERINE HUMPHRY, Department of Physics, Harvard University, Cambridge MA 02138, USA, ARMAND AJDARI, Laboratoire de Physico-Chimie Theorique, ESPCI, Paris, F-75005, France, HOWARD STONE, ALBERTO FERNANDEZ-NIEVES, Division of Engineering and Applied Sciences, Harvard University, Cambridge MA 02138, USA, DAVID WEITZ, Department of Physics and Division of Engineering and Applied Sciences, Harvard University, Cambridge MA 02138, USA — We demonstrate effects of confinement in microfluidic devices with a two phase co-flowing system. When the flow rate of the inner fluid is small compared to the flow rate of the outer fluid, and the resulting width of the inner fluid is smaller than the height of the channel, the inner fluid breaks into droplets, as expected for a three-dimensional system. On the other hand, when the width of the second phase becomes comparable to the height of the microfluidic device, Rayleigh capillary instabilities are suppressed, and the inner fluid forms a jet that does not break, as might be expected for a purely two-dimensional system. We show that by changing the dimensions of the microfluidic channel we can transition from a stable co-flow to drop break-up. The experimental results are compared with of model of this two-phase flow.

#### 9:12AM N21.00007 Playing with Microfluidic Droplets and Actuators, patrick tabeling, espei-enrs,

VALESSA BARBIER, Univ Paris XIII, HERVÉ WILLAIME, ESPCI-CNRS, MMN TEAM — In the lab-on a chips of the future, flows will be handled at the microscale through mazes of microchannels using actuators. Here we concentrate on PDMS based microfluidic systems and we use actuators to introduce localized perturbations on a chip, close to where droplets are formed, i.e. near the intersection of a main and a side channel along which oil and water flows are driven. We observe Arnold tongues and devil staircases leading to the formation of regular or quasiperiodic-like droplets. These behaviors are well accounted for by modelling the system as a non linear oscillator driven by an external forcing. The characteristics of the regimes that are observed depend on the flow-rate conditions. In some range of flow-rates, we show that the droplet sizes can be varied by one order of magnitude by changing the actuation frequency, without modifying the flow-rates. These findings are used to understand the complex behavior of droplet emittors placed in parallel.

#### 9:24AM N21.00008 Droplet Traffic Control at a simple T junction, pascal panizza, wilfried engl,

ANNIE COLIN, LOF/CNRS, ARMAND AJDARI, ESPCI — A basic yet essential element of every traffic flow control is the effect of a junction where the flow is separated into several streams. How do pedestrians, vehicles or blood cells divide when they reach a junction? How does the outcome depend on their density? Similar fundamental questions hold for much simpler systems: in this paper, we have studied the behaviour of periodic trains of water droplets flowing in oil through a channel as they reach a simple, locally symmetric, T junction. Depending on their dilution, we observe that the droplets are either alternately partitioned between both outlets or sorted exclusively into the shortest one. We show that this surprising behaviour results from the hydrodynamic feed-back of drops in the two outlets on the selection process occurring at the junction. Our results offer a first guide for the design and modelling of droplet traffic in complex branched networks, a necessary step towards parallelized droplet-based "lab-on-chip" devices.

#### 9:36AM N21.00009 Manipulation and stretching of bacteria and liposomes by Microfluidics,

EYAL ZUSSMAN, WAEL SALALHA, Faculty of Mechanical Eng., Technion, Israel — Microfluidic technology can be useful in lab-on-a-chip applications of biological assays, environmental monitoring, detection of toxic materials, as well as for assembly of nano- and micro-scale objects into more complex systems. In this work we focused on the orientation of rod-shaped bacteria (Bacillus) by employing shear flow and a high rate elongation flow, and stretching of giant liposomes with diameter size of tens of microns, which can be used as a simplified model for cell behavior. This was achieved by flows of dilute rod-like bacteria and liposome suspensions within a micro-channel by means of a capillary-driven motion. Fluidic alignment situations were tested, firstly by Venturi-like flow which produces a sufficiently converging and diverging flow, and secondly by sink-like flow in a converging microchannel. In the first method we found that the converging part of the flow aligns rod-like bacteria, whereas the diverging part disaligns them, while in the second method the rod-like bacteria can perfectly align along the streamlines. In addition we used the same technology to test liposome deformation while they are flowing through a Venturi-like microchannel. The microfluidics devices were fabricated from poly(dimethylsiloxane) (PDMS) by soft lithographic techniques.

#### 9:48AM N21.00010 Continuous separation of serum from human whole blood within a mi-

**crofluidic device**, JOHN DAVIS, Princeton University, DAVID INGLIS, Princeton University, JAMES STURM, Princeton University, ROBERT AUSTIN, Princeton University — We were able to demonstrate separation of red and white blood cells from their native blood plasma, using a technique known as deterministic lateral displacement. The device takes advantage of asymmetric bifurcation of laminar flow around obstacles. This asymmetry creates a size dependent deterministic path through the device. All components of a given size follow equivalent migration paths, leading to high resolution. A subsequent version of the device will focus on the removal of platelets from whole blood. Samples will be extracted from the microfluidic device and analyzed by conventional flow cytometry.

10:00AM N21.00011 Reversible Dialysis in a Microfluidic Formulator. , SEILA SELIMOVIC, JUNG-UK SHIM, SETH FRADEN, Brandeis University — In order to facilitate the screening of conditions for protein crystallization, we have been using the Microfluidic Formulator chip (Stephen Quake, PNAS Vol. 101, 40 ). This PDMS device allows us to mix up to 40 different reagents and protein solutions. We use this combinatorial approach along with a "drop-on-demand" method whereby we employ on-chip positive displacement pumps to form aqueous droplets containing protein and separate them by plugs of oil. Subsequently, the aqueous drops containing protein are guided by surface tension forces into storage chambers. To control the chemical potential of these sub-nanoliter protein samples, we fabricate reservoirs underneath the storage compartments. A thin PDMS membrane that is permeable to water, but not to protein or salt, separates the reservoirs from the storage chambers. Water can permeate into or out of the stored samples until the chemical potentials of the reservoir and the protein solution are equal leading to protein crystallization in some chambers.

10:12AM N21.00012 A noble microfluidic device for protein crystallizations. , JUNG-UK SHIM, SETH FRADEN, Brandeis University — A high throughput, low volume microfluidic device has been constructed out of poly(dimethylsiloxane) elastomer. We have demonstrated that sub-nanoliter water-in-oil drops of protein solutions of different composition can be rapidly stored in individual wells, which allows screening of 1000 conditions while consuming a total of only 1 microgram protein on a 20 cm<sup>2</sup> chip. This reduction in protein needed for crystal screens allows highthroughput crystallization of mammalian proteins expressed in tissue culture. A significant advance over current microfluidic devices is that each pot is in contact with a reservoir through a dialysis membrane which only water and other low molecular weight organic solvents can pass, but not salt, polymer or amphiphile. This enables the concentration of all solutes in a solution to be reversibly, rapidly, and precisely varied in contrast to current microfluidic methods, which are irreversible. This microfluidic dialysis technology solves a major problem in protein crystallization, the decoupling of nucleation from growth. The device will also be useful for general studies of the phase behavior of protein solutions.

10:24AM N21.00013 Shear induced particle migration in binary colloidal suspensions<sup>1</sup>, DENIS SEMWOGERERE, ERIC R. WEEKS, Emory University, JEFFREY F. MORRIS, City College of New York — We present experimental investigations of the spatial and temporal evolution of particle migration in pressure driven flows of Brownian particle suspensions. Binary suspensions of 1  $\mu$ m- and 3  $\mu$ m-diameter colloidal particles at a variety of concentration ratios and volume fractions are pumped through a 50  $\mu$ m x 500  $\mu$ m rectangular-cross-section capillary tube. Shear rate gradients caused by the resulting parabolic velocity profile drive particles away from the walls towards the center of the channel where the shear rate is lowest. Size segregation is observed. We measure the development of the size segregation by tracking the evolution of the particle concentration down the center of the tube of the small and large sized particles. The flows are directly imaged using high-speed confocal microscopy (up to 300 images/second).

<sup>1</sup>Supported by NSF (DMR-0239109)

 $10:36AM \ N21.00014 \ Using \ permeable \ microcapsules \ to \ deliver \ nanoparticles \ on \ substrates \ , \\ \mbox{ROLF VERBERG, ALEXANDER ALEXEEV, ANNA BALAZS, University of Pittsburgh — We present a novel algorithm to simulate nanoparticles in the presence of a substrate, microcapsules and an externally driven flow. Here, the microcapsules consist of an elastic shell that encloses a fluid with either a dissolved between the microcapsules and an external driven flow. Here, the microcapsules consist of an elastic shell that encloses a fluid with either a dissolved between the microcapsules consist of an elastic shell that encloses a fluid with either a dissolved between the microcapsules consist of an elastic shell that encloses a fluid with either a dissolved between the microcapsules consist of an elastic shell that encloses a fluid with elastic shell that encloses a fluid with either a dissolved between the microcapsules consist of an elastic shell that encloses a fluid with elastic shell that enclo$ chemical component or a suspension of nanoparticles that are small enough to be treated as so-called tracer particles (mutually non-interacting particles without excluded volume). The model couples a lattice-Boltzmann model for the fluid flow, a lattice-spring model for the elastic shell, and a Brownian dynamics model to simulate tracer trajectories. We then apply the model to simulate the release of nanoparticles from a microcapsule as it rolls along a substrate, as well as the subsequent particle adsorption on the wall. We study the effect of flow conditions, reaction kinetics, capsule elasticity, and capsules-substrate interaction on the rate of deposition and the size of the area of deposition at the substrate. The results provide guidelines for designing effective micro-scale delivery systems.

### Wednesday, March 15, 2006 8:00AM - 11:00AM -

Session N26 DBP DFD: Focus Session: DNA and Protein Analysis with Micro and Nano

Fluidics Baltimore Convention Center 323

8:00AM N26.00001 Formation of bi-nanopores in silicon chips1, sang ryul park, hongbo peng, x. s. LING, Brown University — Solid-state nanopores are holes with diameter and length on the order of 20 nm or smaller embedded in an insulating solid membrane. These nanopores have been shown to allow linear translocation of DNA molecules in buffer conditions and can be used as an electronic device for detecting and characterizing nucleic acids and proteins. Here we report a novel method of fabricating bi-nanopores in silicon chips using feedback electrochemical etching. The simplicity and low-cost of our approach, taking advantage of the well-known anisotropic etching behavior of silicon in alkaline solutions, bring solid-state nanopores closer to industrial-scale applications.

<sup>1</sup>This work was supported by the NSF-NIRT program.

8:12AM N26.00002 Fabrication of nanopores in wax using laser-induced shrinking<sup>1</sup>, shanshan wu, SANG RYUL PARK, X. S. LING, Brown University — We developed a simple laser heating induced shrinking technique for making plastic nanopore bio-sensing devices. Our technique is capable of shrinking thermoplastic pores of diameters up to several hundred micrometers to a few nanometers. We have made nanopore devices by applying this technique to Apiezon W wax (thermoplastics) micropores. Our DNA translocation experiments with 48 kilobasepairs (kbp)doublestranded  $\lambda$  DNA ( $\lambda$  dsDNA) have yielded convincing results of the functionality of these devices as biomolecular nanosensors.

<sup>1</sup>This work is supported by an NSF-NIRT (Nanoscale Interdisciplinary Research Team) grant.

8:24AM N26.00003 Ion Valence and Solution Temperature Effects on DNA Translocations in Solid-State Nanopores, JAMES UPLINGER, Physics Department, University of Arkansas, DANIEL FOLOGEA, Physics Department, University of Arkansas, JIALI LI, Physics Department, University of Arkansas — Solid-state nanopore device provides a sensitive and robust environment for single DNA

analysis. When a nanopore is the only participation between two reservoirs filled with an ionic solution and electrical conduction is established any DNA molecule translocation through the nanopore will partially block the open pore current. The current blockage and dwell time depends on both the external parameters, such as applied voltage, ionic strength and on characteristics of the DNA molecule itself, such as the charge and geometry. The properties of the molecule can be modulated by interactions with the ionic solution, and these will produce modifications of the current blockage and translocation time. Here we report on how the DNA translocation signature is modified when: (1) salts of varied valences are used and concentration of the surrounding solution changes; (2) the temperature of ionic solution changes. The mobility and diffusion coefficient of DNA molecule at above conditions are estimated.

8:36AM N26.00004 DNA in nanofluidic devices , ROBERT RIEHN, Princeton University — Nanochannels with a channel cross-section of around 100 nm x 100 nm or less are emerging as a powerful new technique for single-molecule DNA analysis. In these nanochannels, DNA is linearized to a constant fraction of its contour length, and thus spatial locations measured by fluorescence microscopy can be directly related to genomic locations. Because the stretching in nanochannels is caused by lateral confinement, molecules are free to undergo longitudinal fluctuations. Hence, time-averaging over a single molecule is meaningful, and a high resolution can be achieved even using few molecules. We will present how DNA imaging in nanochannels can be applied to common tasks in molecular biology that go beyond simple sizing. In particular, we will discuss the genomic identification of human DNA fragments using fluorescent markers, and how to perform enzymatic reactions, such as restriction mapping using endonucleases, in nanochannels. We will also present our recent progress in the development of "nanoplumbing", that is devices that contain junctions of nanochannels. We will show how device dimensions influence the transport of DNA at those nanochannel junctions, and how those properties can be utilized in the design of devices and exotic materials.

9:12AM N26.00005 Nanoscale electrical detection of DNA, CHIH-KUAN TUNG, Department of Physics, Princeton University, ROBERT REIHN, Department of Physics, Princeton University, LUKAS URBAN, Department of Physics, Urbana-Champaign, ALI YAZDANI, Department of Physics, Princeton University, ROBERT AUSTIN, Department of Physics, Princeton University — We try to detect DNA electrically by different nano-devices, including single-walled carbon nanotubes and platinum nano- wires. We will demonstrate the responses of carbon nanotubes conductance to the exposure to DNA, and ac lock-in measurements across metal nano-wires based on the biochemical properties of the DNA bases. The effects of different bases are also studied, which may provide us a real opportunity to sequence DNA electrically.

9:24AM N26.00006 DNA Translocation Dependence on Ionic Solution Concentration in a Solid-State Nanopore Device , BRIAN THOMAS, Physics Department University of Arkansas Fayetteville Arkansas 72701, DANIEL FOLO-GEA, Physics Department University of Arkansas Fayetteville Arkansas 72701, JIALI LI, Physics Department University of Arkansas Fayetteville, Arkansas 72701 - Our work describes dsDNA translocations through a silicon nitride nanopore subjected to an applied electric field in solutions of different ionic strengths. We demonstrate how the ion concentration affects DNA shielding and, consequently, its effective negative charge. These modifications alter key parameters of the translocation process, such as the dwell time and current drop of the event. In this way, the DNA/salt interaction process can be explored by translocation experiments.

9:36AM N26.00007 DNA size and conformations analysis using a synthetic nanopore, DANIEL 5.50ATV1 1V20.00007 DTVA SIZE and Common and Common analysis using a Synthetic fiamopore, DANIEL FOLOGEA, University of Arkansas, Physics Department, Fayetteville, AR72701, JAMES UPLINGER, University of Arkansas, Physics Department, Fayetteville, AR72701, BRADLEY LEDDEN, University of Arkansas, Physics Department, Fayetteville, AR72701, BRADLEY LEDDEN, University of Arkansas, Physics Department, Fayetteville, AR72701, BRADLEY LEDDEN, University of Arkansas, Physics Department, Fayetteville, AR72701, Department of Molecular and Cellular Biology, Cambridge, MA02138, DANIEL BRANTON, Harvard University, Department of Molecular and Cellular Biology, Cambridge, MA02138, DANIEL BRANTON, Harvard University, Department of Molecular and Cellular Biology, Cambridge, MA02138, JIALI LI, University of Arkansas, Physics Department, Fayetteville, AR72701 — Our work reveals the ability of a synthetic nanopore made in a silicon nitride membrane to discriminate between different conformations and lengths of DNA molecules and presents a comparative analysis with the electrophoretic behavior of the same DNA. Double stranded linear, supercoiled and relaxed form of the same DNA. Jupart restriction fragments as well as single stranded DNA are passed through a synthetic nanopore filled with a buffered tonic solution. of the same DNA, linear restriction fragments, as well as single stranded DNA, are passed through a synthetic nanopore filled with a buffered ionic solution, and a subsequent analysis in terms of current blockage, translocation time and integrated events area shows the analytical ability of such a device. Also, we prove that an intercalating agent increases the temporal resolution by increasing the translocation time up to a factor of two.

9:48AM N26.00008 Microfluidic Protein Crystallography , CARL HANSEN, University of British Columbia — Due to their impressive economies of scale and unique mass transport properties microfluidic devices have become viable technologies for nano-volume protein crystallization screening and growth. In particular, soft microfluidic devices based on multilayer soft lithography (MSL) have been successfully applied to systematic protein solubility studies and efficient nanoliter volume screening by free interface diffusion. While these systems have proven highly effective in identifying crystallization conditions for a large number challenging crystallization targets, realizing the full potential of microscale crystallization requires complementary technologies for crystal optimization and harvesting. In this talk I will briefly review previous studies of protein phase space mapping and crystallization screening, and will present recent work on a microfluidic device which provides a link between chip-based nanoliter volume crystallization screening and structure analysis through "kinetic optimization" of crystallization reactions and direct in situ structure determination. Using this device we demonstrate control over crystal quality, reliable scale-up from nanoliter volume reactions, facile harvesting and cryo-protectant screening, and protein structure determination at atomic resolution from data collected in-chip.

10:24AM N26.00009 Statics and Dynamics of Single DNA Molecules Confined in Nanoslits,

To:224AIVI 1N20.00009 Statics and Dynamics of Single DINA INDECTIES Commed in INTRIOSITIS, PO-KENG LIN, Department of Physics, National Taiwan University, Taipei, Taiwan, CHI-CHENG FU, Institute of Atomic and Molecular Science, Academia Sinica, Taipei, Taiwan, Y.R. CHEN, Graduate Institute of Electronics Engineering and Department of Electrical Engineering, National Taiwan University, Taipei, Taiwan, WUNSHAIN FANN, Institute of Atomic and Molecular Science, Academia Sinica, Taipei, Taiwan, C.H. KUAN, Graduate Institute of Electronics Engineering and Department of Electrical Engineering, National Taiwan University, Taipei, Taiwan — de Gennes provided the scaling predictions for the linear polymer chain trapped in slit with dimension close to the Kuhn length decades ago; however, it has yet to be compared with experiments. We have fabricated nano-slits with vertical dimension similar to the Kuhn length of ds-DNA,  $\sim$  100nm, using standard photolithography. Single DNA molecules with length range from 2 to75 micrometers were successfully inject into the slits and the Brownian motions were imaged by fluorescence microscopy. The distributions of the radius of gyration and the two-dimensional asphericity were measured and it is found that the DNA exhibit highly anisotropic shape distribution. The scaling exponents for the chain extension and the center-of-mass diffusion coefficient will also be discussed exponents for the chain extension and the center-of-mass diffusion coefficient will also be discussed.

10:36AM N26.00010 Slowing down DNA translocation using magnetic and optical tweezers<sup>1</sup>, HONGBO PENG, SHANSHAN WU, SANG RYUL PARK, ANDREW POTTER, X. S. LING, Brown University — Electric-field driven DNA translocation through nanopores can be exploited for DNA sequencing and other applications. However, the DNA translocation under normal patch-clamp-type measurement is too fast to allow detailed measurements of individual or few nucleotides. We propose a concept to slow down the DNA translocation through the nanopore by using magnetic (or optical) tweezers. The 3' end of a single-strand DNA can be attached to a streptavidin-coated magnetic bead through a single biotin molecule. During DNA translocation, the 5' end of DNA will be electrophoretically drawn through the nanopore to the *trans* side while the 3' end of DNA stays in the *cis* side with the magnetic bead. A set of permanent magnets or electric coils can be used to generate a magnetic field gradient large enough to pull the bead, hence the DNA out of the nanopore. The net force on the magnetic bead will determine this back-translocation speed. By carefully tuning the magnetic field gradient and the voltage bias on the nanopore, one can make the back-translocation much slower than the conventional forward-translocation in which case the DNA is driven only by the electric force. We will report our experimental design as well as the preliminary results.

<sup>1</sup>This work was supported by NSF-NIRT.

#### 10:48AM N26.00011 Patterned Periodic Nanofilter Array for Continuous-Flow Bimolecular

Separation, JIANPING FU, Department of Mechanical Engineering, MIT, JONGYOON HAN, Department of Electrical Engineering and Computer Science, Division of Biological Engineering, MIT — We present an experimental study on sieving process of small biomolecules (i.e., proteins and small DNAs) in one- and two-dimensional periodic arrays of nanofilter. The nanofilters served as artificial sieves with precise pore size characterization and showed exceptional size selectivity and separation efficiency from the periodicity of the environment. A kinetic model is developed to explain the electrophoretic drift of charged molecules across periodically modulated free energy landscapes. Further experimental evidence shows the crossover from Ogston-like sieving to entropic trapping mechanism depending on nanofilter thickness and on electric field strength. We also demonstrate continuous-flow biomolecule separation with a device containing of two-dimensional periodic nanofilter arrays. The interaction between migrating molecules and the two-dimensional physical landscapes cause molecules of different sizes to follow radically different paths leading to separation. Continuous-flow fractionations of small DNA molecules (50bp-766bp) as well as SDSprotein complexes (11kDa-200kDa) were achieved in about 5 minutes with a resolution of 10%. By virtue of its gel-free and continuous-flow operation, this device suggests himself a key component to an integrated biomolecule sample preparation and analysis microsystem.

## Wednesday, March 15, 2006 11:15AM - 2:15PM –

Session P5 DFD: Shedding Light on the Enigma of the Transition to Turbulence in Pipes and other Shear Flows Baltimore Convention Center 309

11:15AM P5.00001 The Transition to and from Turbulence in a pipe<sup>1</sup>, TOM MULLIN, DFD — A discussion of experimental investigations of the stability of flow along a pipe will be given. The transition to turbulence is catastrophic when a well-defined amplitude of injected perturbations is exceeded. The stability threshold scales inversely proportional to the Reynolds number, Re, with a sharp cut off at low Re values. On the other hand, the decay from the turbulent state exhibits systematic exponential behavior with diverging timescales which are indicative of critical behavior. The long transients contain spatio-temporal coherence which suggest connections with recent theoretical developments.

<sup>1</sup>Support from EPSRC 'Senior Fellowship'. Joint work with J. Peixhino.

11:45AM P5.00002 Transient growth and subcritical transition in shear flows, DAN HENNINGSON, KTH Mechanics — The possibility for disturbance growth in shear flows which are linearly stable is discussed, and it is shown that a necessary condition is that the underlying linear operator is non-normal, i.e. that it is associated with non-orthogonal eigenfunctions. Since the non-linear terms are conservative it is only by utilizing linear growth mechanisms associated with the non-normal linearized operator that energy growth is possible also for subcritical finite amplitude disturbances. The non-normal effects are manifested in the possibility for large transient growth of the disturbance energy, large response to forcing and large sensitivity of the eigenvalues. The optimal transient growth and response to forcing are calculated as the norm of the matrix exponential and resolvent, respectively. The optimal disturbances are streamwise vortices and the optimal responses are streaks of high and low velocity in the streamwise direction. These flows structures are prevalent in all subcritical transitional shear flows, including pipes and channels. It is shown by direct numerical simulations that transition scenarios initiated by the optimal disturbances have low transition thresholds. The dependence of the thresholds on the Reynolds number is also presented. Finally, extensions of the transient growth concept to more complex flows are discussed and examples of its use given.

#### 12:15PM P5.00003 Self-Sustaining Process and Exact Coherent Structures in Shear Flows,

FABIAN WALEFFE, Depts. of Mathematics and Engineering Physics, University of Wisconsin-Madison — The Self-Sustaining Process (SSP) is a weakly nonlinear theory of a fundamental three-dimensional nonlinear process in shear flows. It is the basic mechanism that enables enhanced momentum transport and the redistribution of the mean shear energy into smaller scales and, ultimately, turbulent motions. I will briefly review the 40 years of observations of streaks and coherent structures in the near wall region of turbulent shear flows that led to the formulation of the SSP theory. A primary impact of the SSP, besides providing some level of mechanistic understanding, has been to provide a method to calculate unstable traveling wave solutions of the Navier-Stokes equations. This approach has now been successfully carried out in all canonical wall-bounded shear flows with stress as well as velocity boundary conditions. The traveling waves thus obtained show striking similarity with the observed near-wall coherent structures, earning them the name of 'exact coherent structures'. Furthermore, those unstable waves have been shown to capture basic statistics of turbulent flows remarkably well, thereby providing hope for a quantitative theory of turbulence over smooth walls. The traveling waves come in many kinds: small scales, large scales and multi-scales. The asymptotics of the large scale traveling waves are the Reynolds number goes to infinity is remarkably simple and confirms the asymptotic validity of the SSP. These large scale coherent states may yield a new promising target for the control of turbulence in shear flows.

#### 12:45PM P5.00004 Travelling waves in pipe flow and their relevance for transition to turbu-

**lence**, RICH KERSWELL, Bristol University — The problem of understanding the nature of pressure-driven fluid flow through a circular straight pipe remains one of the oldest problems in fluid mechanics. The steady, unidirectional parabolic (laminar) flow solution named after Hagen (1839) and Poiseuille (1840) is linearly stable yet temporally and spatially disordered 3-dimensional (turbulent) solutions can easily be triggered at sufficiently large flow rates (Reynolds 1883). In contrast with Rayleigh-Benard convection where transition to turbulence proceeds along an orderly sequence of bifurcations at well-defined values of the thermal driving, the transition in a pipe is abrupt, dependent on the level of ambient disturbances in the system and, at least close to the threshold flow rate, transient. The recent discovery of travelling wave solutions (which represent saddle points in phase space) in this system has at last provided a theoretical stepping stone towards rationalizing the transition process. We will discuss the structure of these waves as well as evidence of their relevance during the transition process.

#### 1:15PM P5.00005 Two scenarios for dynamics of perturbations in pipe Poiseuille flow, ANATOLI

 $TUMIN^1$ , The University of Arizona — Two experiments on perturbations in circular pipe flows and their possible theoretical interpretations are discussed to illustrate complexity of the problem. The experimental data by A. Kaskel (1961) are discussed within the framework of spatial transient growth theory, and we argue that the phenomenon of transient growth was observed in the pipe-flow experiments. Another experiment (Eliahou et al, 1998) illustrates how weak streamwise vortices provide instability of the secondary disturbances which, in turn, amplify the steady vertical structures. The latter is consistent with the self-sustaining process scenario. These examples, and more recent DNS and experimental studies represent typical controversies that arise in the study of complex systems.

<sup>1</sup>In collaboration with Prof. Eli Reshotko, CWRU

1:45PM P5.00006 Edge of chaos in the transition to turbulence, BRUNO ECKHARDT, Philipps Universität Marburg — We study the boundary of the laminar region near the onset of turbulence. Approaching the boundary from the laminar side, the lifetime of perturbations increases, diverges when the boundary is reached, and varies chaotically for larger amplitudes. In the chaotic region, lifetimes vary sensitively with amplitude, consistent with the strange saddle picture of the turbulence proposed earlier. The trajectory on the edge between the laminar and chaotic regions is asymptotic to a single well defined state, essentially independent of the type of perturbation. The edge then becomes the stable manifold of this structure. In the case of a model shear flow, the edge states are simple or period doubled or chaotic trajectories. The case of pipe flow shows less variability and the edge state seems to remain close to a state with simple vortical structure.

This is joint work with T.M. Schneider (U Marburg), J.D. Skufca (Clarkson U) and J. Yorke (U Maryland).

#### Wednesday, March 15, 2006 11:15AM - 2:15PM – Session P8 DFD GSNP: Focus Session: Jets, Shocks & Splashes Baltimore Convention Center 314

11:15AM P8.00001 The secret of splashing: interplay of air and roughness , LEI XU, University of Chicago — We studied splashing on both smooth and rough dry surfaces using high speed photography. For smooth substrates, a striking phenomenon is observed: splashing can be completely suppressed by decreasing the pressure of the surrounding gas. The threshold pressure where a splash first occurs is measured as a function of the impact velocity and found to depend on the molecular weight of the gas and the viscosity of the liquid. Both experimental scaling relations support a model in which the compressibility of the gas is responsible for creating the splash[1]. For the case of rough substrates, we systematically varied both the surface roughness and the pressure of the surrounding gas and found two distinct contributions to a splash. One is caused by air and has the same characteristics as the "coronal" splash observed on smooth substrates. A second, "prompt" splash, contribution is caused by surface roughness. We have also measured the size distribution of the droplets emitted from a splash. For a smooth surface, a broad distribution of droplet sizes is found at high gas pressures. As the gas pressure is lowered towards the splash/no-splash transition the distribution gets more and more peaked at a characteristic size. For a rough surface, the distribution is strongly correlated with the surface roughness. [1] L Xu, W W Zhang and S R Nagel, Phys. Rev. Lett. 94, 184505 (2005)

11:51AM P8.00002 Statistical Mechanics of a Geophysical Jet<sup>1</sup>, EMILY CONOVER, J.B. MARSTON, Brown University — We investigate the equal-time statistics of an equatorial jet in a two-dimensional quasi-geostrophic model of a planetary atmosphere on a rotating sphere<sup>2</sup>. Potential vorticity is advected by the barotropic flow and at the same time relaxes towards the zonal shear flow of an underlying equatorial jet. A transition to turbulence occurs at sufficiently slow relaxation rates. Statistics accumulated by direct numerical simulation<sup>3</sup> are compared to those obtained by a simple cumulant expansion. We study rigorous upper bounds on the instability size<sup>4</sup> and discuss the limitations of the cumulant expansion.

<sup>1</sup>Supported in part by NSF DMR-0213818.

<sup>2</sup>R. S. Lindzen, A. J. Rosenthal, and R. Farrell, J. Atmos. Sci. 40, 1029 (1983).
 <sup>3</sup>Akio Arakawa, J. Comp. Phys. 1, 119 (1966).
 <sup>4</sup>T. G. Sharkard, J. Eheid, Math. 102, 201 (1983).

<sup>4</sup>T. G. Shepherd, J. Fluid. Mech. **196**, 291 (1988).

12:03PM P8.00003 High-Speed X-ray Investigation of Granular Jets<sup>1</sup>, JOHN ROYER, ERIC CORWIN, ANDREW FLIOR, BRYAN CONYERS, MARIA-LUISA CORDERO, MARK RIVERS, PETER ENG, HEINRICH JAEGER, James Franck Institute, The University of Chicago — When a heavy sphere is dropped onto a bed of loose, fine sand, a large, focused jet of sand shoots upward.<sup>2</sup> <sup>3</sup> Experiments at reduced air pressure reveal that the jet in fact consists of two components: a wispy, thin jet that varies little with pressure followed by a thick air-pressure-driven jet <sup>4</sup>. To observe the initial stages of jet formation inside the granular bed, we employed x-ray radiography using the high-intensity beams available at the Advanced Photon Source. This technique allowed us to image the motion of the sphere and the evolution of the void left behind it at frame rates up to 6600 frames per second. The x-ray movies reveal that gravity-driven collapse produces the initial, thin jet, while the compression of an air pocket trapped below the surface drives up the thick jet. We also find that the interstitial air alters the compressibility of the sand bed. In vacuum a visible compaction front precedes the ball, while at atmospheric pressure the sand flows out of the way of the ball, behaving more like an incompressible fluid.

<sup>1</sup>This work was supported by NSF and DOE.
<sup>2</sup>Thoroddsen, S. T. and Shen, A. Q. Phys. Fluids 13, 4-6 (2001).
<sup>3</sup>Lohse, D. et al. Phys. Rev. Lett. 93 (2004).
<sup>4</sup>Royer, J. et al. Nature Physics, December 2005.

12:15PM P8.00004 Measurement of Stopping Force in Low Velocity Impact Cratering, JOSEPH AMATO, MICHAEL NITZBERG, Colgate University — The time dependent stopping force on a ball dropped into a granular medium has been measured using an accelerometer embedded within the ball. The velocity dependence of the force shows two distinct behaviors: (1) for impacts with large (200  $\mu$ m) irregularly shaped sand particles,  $F(v) \propto v^{1/2}$ ; for impacts with 100  $\mu$ m spherical glass beads,  $F(v) \propto (v - v_0)$ . The accelerator apparatus yields reproducible, low noise data that reveals peculiar features such as a downward acceleration pulse just before the ball comes to rest.

12:27PM P8.00005 Giant bubble-pinchoff<sup>1</sup>, DETLEF LOHSE, University of Twente — Self-similarity has been the paradigmatic picture for the pinch-off of a drop. Here we will show through high-speed imaging and boundary integral simulations that the inverse problem, the pinch-off of an air bubble in water, does not obey self-similarity (of the first kind): A disk is quickly pulled through a water surface, leading to a giant, cylindrical void, which at collapse creates an upward and a downward jet. The neck radius h(tau) of the void does NOT scale with the inertial power law exponent 1/2 (i.e., does not obey "Rayleigh-scaling"). This is due to a second length-scale, the inverse curvature of the void, which follows a power-law scaling with a different exponent. Only for infinite Froude numbers the scaling exponent 1/2 is recovered. In all cases we find the void-profile to be symmetric around the minimal void radius up to the time the airflow in the neck deforms the interface.

<sup>1</sup>In collaboration with Raymond Bergmann, Devaraj van der Meer, Mark Stijnman, and Andrea Prosperetti, University of Twente.

1:03PM P8.00006 Nano-liquid bridges in ambient conditions , WEI KANG, UZI LANDMAN, School of Physics, Georgia Institute of Technology, Atlanta, GA 30332 — The dynamics of nano-liquid bridges in an ambient gaseous environment is studied using molecular dynamics simulations. Under these conditions new behavior close to break-up is found, compared to the behavior in vacuum. The probability for appearance of a long-thread structure close to pinch-off, versus the appearance of a double-cone profile in vacuum, depends on the density of the ambient gas. The stochastic lubrication equation that has been introduced by Moseler and Landman [1] for the case of break-up in vacuum is modified to include an additional term representing the effect of the ambient gas. Numerical integration of the modified stochastic lubrication equation shows good agreement with the molecular dynamics simulations. [1] M. Moseler and U. Landman, Science 289, 1165(2000).

1:15PM P8.00007 Splashing on dry, smooth inclined surfaces , JAMES BIRD, Harvard University, DAVID WEITZ, Harvard University, HOWARD STONE, Harvard University, MICHAEL BRENNER, Harvard University — We investigate splashing of drops on dry, smooth inclined surfaces. The asymmetry of the impact leads to an azimuthal variation of the ejected rim. We show that under certain conditions only part of the rim splashes. A model for the azimuthal splash threshold is compared both with the data and with existing splash criteria.

1:27PM P8.00008 Levitation of Falling Spheres in Stratified Fluids<sup>1</sup>, RICHARD MCLAUGHLIN, ROBERTO CAMASSA, BYRON HUFF, RICHARD PARKER, University of North Carolina, UNC RTG FLUIDS GROUP COLLABORATION — The motion of sphere's falling under the influence of gravity is a classical problem dating back to Galileo and earlier. How a falling body additionally interacts with its environment is an equally challenging problem and involves strong coupling between the body and fluid via hydrodynamic drag. We present new phenomena<sup>2</sup> concerning the motion of a sphere falling through a sharply stratified (two layer) fluid in which the falling heavy body stops and reverses its direction (bounces) before ultimately returning to descent. Shadowgraph imaging shows the physics responsible for this surprising motion is a coupling between the body and the ambient boundary layer fluid, which is endowed with a negative potential energy as it is drawn into the lower layer, forming a rising turbulent plume. The hydrodynamic coupling between the sphere and this plume temporarily arrests the motion, even causing the bead to rise back through the transition layer. We present measurements of this trapping phenomena, and report the long residence times in which the sphere is trapped within the transition layer as a function of the bottom layer fluid density field for an array of different sized spheres. <sup>2</sup> N. Abaid, D. Adalsteinsson, Akua Agyapong, and R. M. McLaughlin, "An Internal Splash: Falling Spheres in Stratified Fluids," Physics of Fluids, 16, no. 5, 1567-1580, 2004.

<sup>1</sup>RTG NSF DMS-0502266

1:39PM P8.00009 Sodium luminescence from laser-induced bubbles in salt water<sup>1</sup>, sonny vo. TIM HSIEH, HAN-CHING CHU, GARY WILLIAMS, UCLA — Luminescence from collapsing laser-induced bubbles in salt water (up to 1M NaCl) has been studied. We find a new emission pulse from the 589 nm sodium line that arrives about 50 ns prior to the main blackbody luminescence pulse. This may be related to the dynamics of the compressional heating process in the bubble. We have also noticed in the salt water that the time duration of the blackbody pulse is reduced by up to 30% from the duration in pure water, and this has been observed in several other alkali salt solutions.

<sup>1</sup>Work supported in part by the NSF, DMR 01-31111

1:51PM P8.00010 The dynamics of a flexible loop in a high-speed flow , SUNGHWAN JUNG, AML, Courant Inst., New York Univ., KATHLEEN MARECK, AML, Courant Inst., New York Univ., MICHAEL SHELLEY, AML, Courant Inst., New York Univ., JUN ZHANG, AML, Courant Inst., New York Univ. — We study the behavior of an elastic loop in a fast-flowing soap film. The loop is wetted into the film and is held fixed at a single point against the oncoming flow. We interpret this system as a 2D closed flexible body moving in a quasi-2D flow. The loop is deformed by the flow, and this coupled fluid-structure system shows bi-stability: stationary and oscillatory. In its stationary state, the loop essentially remains motionless and its wake is a von Kármán vortex street. In its oscillatory state, the loop sheds two vortex dipoles within each oscillation period. The frequency of oscillation of the loop is linearly proportional to the flow velocity.

2:03PM P8.00011 Superfluid-like shock waves in nonlinear optics, wenjie wan, jason w. fleischer, Princeton University — It is well-known, but often underappreciated, that condensate dynamics has analogies with nonlinear light propagation in optics. In both cases, a single, macroscopic wavefunction describes the coherent wave behavior of interest. Here, we take advantage of this correspondence and examine superfluid-like spatial shock waves by propagating coherent light through a nonlinear crystal. We report the observation of both 1D and 2D shock waves, their nonlinear behavior as a function of intensity, and double-shock wave collisions. Analytical calculations and numerical simulations show excellent agreement with the experimental results. The fine structures and features observed here match similar observations in previous shock studies using superfluids and BEC, obtained in this case in a table-top apparatus, without the need for vacuum isolation, ultracold temperatures, etc. Moreover, the inherent optical advantages of easy control of the wavefunction input and direct imaging of the output make us optimistic that the nonlinear photonic systems described here will lay the foundation for a whole series of condensate-inspired experiments, many of which would be difficult (if not impossible) to perform in the corresponding condensed matter environments.

## Wednesday, March 15, 2006 11:15AM - 2:03PM –

Session P21 DFD: Microfluidic Physics III Baltimore Convention Center 318

11:15AM P21.00001 Multi-Point Holographic Micro-Velocimetry, roberto di leonardo, infm-cnr Dipartimento di Fisica, Universita' di Roma "La Sapienza", Roma, Italy, JONATHAN LEACH, Department of Physics and Astronomy, University of Glasgow, Glasgow, Scotland, HASAN MUSHFIQUE, Department of Electrical Engineering, University of Glasgow, Scotland, JOHN COOPER, Department of Electrical Engineering, University of Glasgow, Glasgow, Scotland, GIANCARLO RUOCCO, INFM-CNR Dipartimento di Fisica, Universita' di Roma "La Sapienza", Roma, Italy, MILES PADGETT, Department of Physics and Astronomy, University of Glasgow, Glasgow, Scotland — We show how holographic optical trapping can be used for the multi-point measurement of fluid flow in microscopic geometries. An array of microprobes can be simultaneously trapped and used to map out the fluid flow in a microfluidic device. The optical traps are alternately turned on and off such that the probe particles are displaced by the flow of the surrounding fluid and then re-trapped. The particles' displacements are monitored by digital video microscopy and directly converted into velocity field values. The validity of the technique is demonstrated for the case of the flow around a spinning sphere and the flow at the outlet of a micro-channel field values. The validity of the technique is demonstrated for the case of the flow around a spinning sphere and the flow at the outlet of a micro-channel.

#### 11:27AM P21.00002 A Hybrid Microwave Source and Irradiator for Biological Lab On a Chip

Applications. , DAVID ISSADORE, Harvard University, Department of Engineering and Applied Sciences, TOM HUNT, KRISTI ADAMSON, Harvard University, Physics, ROBERT WESTERVELT, Harvard University, Department of Engineering and Applied Sciences, RICK ROGERS, Harvard Medical School Using a standard lithographic process, we have built a hybrid microwave irradiator for use in microwave enhanced chemistry and localized, rapid heating. The device combines a 100mW microwave source with a near field antenna to produce an entirely on-chip system for delivering microwave energy into a thin( $<100\mu$ m) layer above a substrate. The antenna utilizes a serpentine wire pattern to produce a thin layer of intense microwave electromagnetic field intensity that falls off exponentially in distance away from the substrate. The device, including RF electronics, was built on a standard 1" by 3" glass slide, and several antenna pixel sizes are tested for Biological Lab On a Chip Applications. This work is made possible by the NSEC NSF grant PHY-0117795.

11:39AM P21.00003 Simulations of Contact Line Motion in Partially Miscible Fluids, SHENGFENG CHENG, Dept of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218, USA, COLIN DENNISTON, Dept of Applied Mathematics, The University of Western Ontario, London, Ontario, Canada N6A 5B8, MARK ROBBINS, Dept of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218, USA — We report on extensive molecular-dynamics simulations of contact line motion in partially miscible fluids confined between two solid walls and sheared in a Couette geometry. Our results show that diffusion alone cannot remove the stress singularities at the contact line or lead to no-slip boundary conditions on the fluid velocity. Computed velocity fields show that there is a substantial drop of the fluid velocity near the contact line, which is associated with the gradient of the fluid-solid interfacial tension in the same region. However, the fluid velocity does not fall to zero at the contact line, in contrast to the case where fluids are immiscible. The nonzero velocity leads to a net advective flux across the fluid-fluid interface, which is balanced by the diffusive flux induced by the concentration gradient. The advective and diffusive fluxes across the interface are only significant in the very first layer of fluid atoms.

#### 11:51AM P21.00004 Macromolecular Liquids Slip Over Solid Surfaces: Experimental Studies

of the Slip Length<sup>1</sup>, KARIN JACOBS, RENATE FETZER, Saarland University, Dept. of Experimental Physics, 66041 Saarbruecken, Germany We present a novel method to asses the slip length and viscosity of thin films of highly viscous Newtonian liquids. We quantitatively analyze dewetting fronts of low molecular weight polystyrene melts on Octadecyl- (OTS) and Dodecyltrichlorosilane (DTS) polymer brushes [1]. Using a thin film (lubrication) model derived in the limit of large slip lengths, we can extract slip length and viscosity of films with thicknesses between 50 nm and 230 nm and temperatures above the glass transition. We find slip lengths from 100 nm up to 1 micron on OTS and between 300 nm and 10 microns on DTS covered silicon wafers. The slip length decreases with temperature. The obtained values for the viscosity are consistent with independent measurements [2]. [1] R. Fetzer, K. Jacobs, A. Muench, B. Wagner, T.P. Witelski, Phys. Rev. Lett. 95, 127801 (2005) [2] R. Fetzer, K. Jacobs, M. Rauscher (to be published)

<sup>1</sup>Priority Program SPP 1146 "Nano- and Microfluidics" of the German Science Foundation

12:03PM P21.00005 Source of Shear Dependent Slip at Liquid/Solid Interfaces, NIKOLAI PRIEZJEV<sup>1</sup>,

Michigan State University, SANDRA TROIAN<sup>2</sup>, Princeton University — Slippage at liquid/solid interfaces can strongly influence transport behavior in microand nanoscale systems. Previous molecular dynamics (MD) studies of simple and polymeric fluids subject to planar shear at small Reynolds number have shown that the slip length increases as a power law in the shear rate for moderate to high values. The corresponding boundary condition provides a new generalization of the Navier slip law. In this talk, we examine what physical mechanism is responsible for the shear rate exponent by focusing on the collision events between the fluid particles in the first layer and the adjacent wall particles comprising a crystalline surface. By examining the interfacial frictional force as a function of the fluid sliding velocity, we recover similar behavior as inherent in the generalized slip condition and determine that the dominant frictional response stems from the repulsive part of the Lennard-Jones interaction potential. A reduced kinetic model describing the scattering of a single molecule with a given slip velocity along a crystalline surface helps explain the saturation in the frictional force at large sliding velocities. These results elucidate how different is the slip behavior at liquid/solid interfaces from that observed in rarefied gases.

<sup>1</sup>Dept. Mechanical Engineering <sup>2</sup>Dept. Chemical Engineering

12:15PM P21.00006 Apparent Slip at Hydrophilic Surface: Flow Profile within 1 nm from the Surface, SUNG CHUL BAE, STEPHEN ANTHONY, STEVE GRANICK, Departments of Materials Science and Engineering, of Chemistry, of Physcis, University of Illinois — Fluid dynamics within small channels draws great interest due to the development of microfluidic devices, yet details about flow immediately at a solid surface remain too vague. Here, by using fluorescence energy transfer (FRET and fluorescence quenching) approaches, we measured the flow rate of fluorescence quencher molecules within 1 nm from the quartz surface within a specially-designed microfluidic device. In parallel, we have simulated the flow dynamics at the surface, in order to separate cleanly the actual near-surface velocity from the confounding effects of near-surface diffusion.

12:27PM P21.00007 Slip versus Friction : Modifying the Navier condition , EVANGELOS KOTSALIS, ETHZ, JENS WALTHER, ETHZ & TU Denmark, PETROS KOUMOUTSAKOS, ETHZ — The modeling of fluid-solid interfaces remains one of the key challenges in fluid mechanics. The prevailing model, attributed to Navier, defines the fluid "slip" velocity as proportional to the wall shear and a parameter defined as the slip length. Several works have in turn proposed models for this slip length but no universal model for the slip velocity has been accepted. We present results from large scale molecular dynamics simulations of canonical flow problems, indicating, that the inadequacy of this classic model, stems from not properly accounting for the pressure field. We propose and validate a new model, based on the fluid elements will lead to their acceleration which in turn may result in a slip velocity at the interface. We formulate the slip velocity in terms of fluid-solid friction  $F_f$  and propose a generalized boundary condition:  $F_f = F_s + F_p = \lambda_u u_s + \lambda_p p$  where p denotes the pressure, and  $\lambda_u$  and  $\lambda_p$  the viscous and static friction coefficients, for which universal constants are presented. We demonstrate that the present model can overcome difficulties encountered by the classical slip model in canonical flow configurations.

12:39PM P21.00008 Slip and Air-Entrainment at Water-Solid Interfaces , YINGXI ELAINE ZHU, PRASAD SARANGAPANI, Department of Chemical and Biomolecular Engineering, University of Notre Dame, ASHIS MUKHOPADHYAY, Wayne State University — A number of recent studies performed with water flow past hydrophobic microchannels have reported the existence of 'slip' at wall and suggested the existence of the interfacial gas layer as the underlying mechanism for the slip motion, yet the details are much disputed. We combine microscopy and advanced laser spectroscopy to directly and non-invasively detect the interfacial gas layer in flowing water past micro/nano-channels whose surface chemistry and gap spacing are varied. We observe that the dimension of the gas layer strongly depends on surface hydrophobicity and flow rates. Surprisingly, we have also observed the slip motion of water over hydrophilic surfaces with a strong dependence on liquid-loading conditions. We propose a mechanistic theory about air-entrainment that can account for our observations to elucidate the origin of the gas formation at water-solid interface and its consequence on slip motion.

12:51PM P21.00009 Rheology of sub-nanometer thick water films , TAI-DE LI, ROBERT SZOSZKIEWICZ, ELISA RIEDO, SCHOOL OF PHYSICS, GEORGIA INSTITUTE OF TECHNOLOGY TEAM — Knowing the behavior of water in small volumes is essential for the understanding of many processes in biology, tribology, and geophysics. Water under nano-confinement plays a crucial role in biological and technological systems. Here, we report an experiment in which an atomic force microscope tip approaches a flat solid surface in purified water, while small lateral oscillations are applied to the tip. The normal and lateral forces acting on the tip are measured directly and simultaneously as a function of water thickness. We find that, for hydrophilic surfaces, oscillatory solvation forces are present in the last four adjacent water layers where the dynamic viscosity is measured to grow up orders of magnitude in respect to bulk water. The same effects are present for atomically smooth surfaces and slightly rough surfaces. Oscillatory solvation forces have been detected also when the confining flat surface was hydrophobic.

1:03PM P21.00010 Wetting morphologies on surfaces nanopatterned with chemical stripes<sup>1</sup>, ANTONIO CHECCO, OLEG GANG, BENJAMIN M. OCKO, Condensed Matter Physics and Materials Science Dept. Brookhaven Natl. Laboratory, SOFT MATTER GROUP TEAM — Here we investigate the wetting of simple, volatile liquids on model chemical nanopatterns created using Local Oxidation Nanolithography. This technique makes use of a biased, metallic AFM tip to locally oxidize the methyl-terminations of a self-assembled monolayer (octade-cylthrichlorosilane) into carboxylic acid termination[1]. With this method we have realized parallel, 50 to 500 nm wide, wettable stripes (carboxylic) embedded into a non-wettable (methyl) surface. Several organic (polar, non-polar), volatile liquids have been condensed onto the nanopatterned surface and the resulting wetting morphologies have been studied in-situ by using an environmental AFM. Initially the liquid only condenses on the wettable stripes to form a thin liquid film. Close to saturation the liquid morphology becomes drop-like. Eventually, when more and more liquid is condensed on the stripes, the liquid drops may "spill over" into the non-wettable spacer so that neighboring lines merge and undergo a "morphological wetting transition". For all of these regimes we show that long-range forces are relevant to nanoliquid "shape". Results will be compared with those of Density Functional Theory.[1] R. Maoz, S. Cohen, and J. Sagiv, Adv. Mater. **11**, 55 (1999)

<sup>1</sup>This work is supported by the U.S. DOE under contract No. DE-AC02-98CH10886

1:15PM P21.00011 Self-propelled film-boiling liquids , HEINER LINKE, MICHAEL TAORMINA, BENJAMIN ALEMAN, LAURA MELLING, COREY DOW-HYGELUND, RICHARD TAYLOR, University of Oregon, MATTHEW FRANCIS, University of Sydney — We report that liquids perform self-propelled motion when they are placed in contact with hot surfaces with asymmetric (ratchet-like) topology. Millimeter-sized droplets or slugs accelerate at rates up to 0.1 g and reach terminal velocities of several cm/s, sustained over distances up to a meter. The pumping effect is observed when the liquid is in the film-boiling regime, for many liquids and over a wide temperature range. We propose that liquid motion is driven by a viscous force exerted by vapor flow between the solid and the liquid. This heat-driven pumping mechanism may be of interest in cooling applications, eliminating the need for an additional power source.

1:27PM P21.00012 Ratcheting motion of capsules on tailored substrates , ANNA C. BALAZS, KURT A. SMITH, ALEXANDER ALEXEEV, ROLF VERBERG, University of Pittsburgh — We study the motion of microcapsules on attractive surfaces. The capsules, modeled as fluid-filled elastic shells, represent polymeric microcapsules or biological cells. Certain periodic surface patterns give rise to directed capsule motion for a symmetric energy input, such as an oscillatory shear flow. We use a numerical model which integrates a lattice spring representation of the capsule shell and the substrate with a lattice Boltzmann representation for the fluid regions. We consider, as a surface pattern, a series of asymmetric ramps. The minimum shear necessary to drive a capsule "forward" over one ramp is less than that needed to drive the capsule "backward" over a ramp. We show under what conditions it is possible to move the capsule forward, in a ratcheting motion, via an imposed oscillatory flow. These patterned surfaces could be used to control capsule motion precisely, based on flow and surface properties. They coud also be used to efficiently sort capsules based on their size or material properties.

1:39PM P21.00013 Electrowetting for Digital Microfluidics , TOM HUNT, KRISTI ADAMSON, Harvard Physics, DAVID ISSADORE, ROBERT WESTERVELT, Harvard Division of Engineering and Applied Science — Droplet based chemistry promises to greatly impact biomedical research, providing new avenues for high throughput, low volume assays such as drug screening. Electrowetting on Dielectric (EWOD) is an excellent technique for manipulating microscopic drops of liquid. EWOD uses buried electrodes to locally change the surface energy between a droplet and a substrate. We present microfabricated devices for moving droplets with EWOD. One example of such a device consists of a series of 16 interdigitated electrodes, decreasing in size from 1mm to 20 microns. Each electrode is addressable by an independent, computer controlled, high voltage supply. This work made possible by a gift from Phillip Morris and the NSEC NSF grant PHY-0117795.

1:51PM P21.00014 Surface mediated liquid transport on nanotube, MIN-FENG YU, Univ. of Illinois at Urbana-Champaign, KYUNGSUK YUM — The surface mediated liquid transport on nanotubes was studied using a nanotube-based liquid transport system. Microscale liquid droplets were formed and transferred to nanotubes using the liquid transport system integrated with a nano-manipulator. If the spreading parameter S is larger than a threshold value  $S_c$ , the liquid spontaneously flows out of the liquid droplet through a thin precursor film formed along the nanotube surface. The liquid transport on nanotube surfaces was studied *in situ* by measuring the volume flow rate which was obtained from a direct observation of the droplet. The flow rate dependence on the size of nanotubes and surface energy were also investigated. The surface mediated liquid transport phenomenon can be exploited for the development of nanoscale liquid transport system for nanofabrication and nanoscale devices for biological and chemical applications. Reference: Kyungsuk Yum and Min-Feng Yu, Surface-mediated liquid transport through molecularly thin liquid films on nanotubes, Phys. Rev. Lett. 95, 186101 (2005)

#### Wednesday, March 15, 2006 2:30PM - 5:30PM – Session R8 DFD: Monolayers, Membranes & Microemulsions Baltimore Convention Center 314

2:30PM R8.00001 Theory of Myelin Coiling , JUNG-REN HUANG, THOMAS WITTEN, University of Chicago — We propose a new model to explain coiling of myelins composed of fluid bilayers. This model allows the bilayer cylinders of a myelin to be non-coaxial and the bilayer lateral tension to vary from bilayer to bilayer. Our calculations suggest that a myelin would bend or coil to lower its free energy when the bilayer lateral tension is sufficiently large. The proposed coiling mechanism is in a sense similar to the classical Euler buckling of a thin elastic rod subject to axial compression. The analysis of a simple two-bilayer case shows that a bilayer lateral tension of about 1 dyne/cm can easily induce coiling of myelins of typical lipid bilayers. This model signifies the importance of bilayer lateral tension in determining the morphology of myelinic structures.

2:42PM R8.00002 Curvature condensation and twinning in an indented elastic shell, MOUMITA DAS, ASHKAN VAZIRI, Harvard University, ARSHAD KUDROLLI, Clark University, L. MAHADEVAN, Harvard University — We study the formation of a localized geometrical defect and its evolution in an elastic shell using a combination of experiment and numerical simulation. We find that as a symmetric localized indentation on a semi-cylindrical shell increases, there is a transition from a global mode of deformation to a localized one which leads to the condensation of curvature along a parabolic crease along the line of symmetry. Further indentation leads to a twinning phenomena wherein the crease bifurcates into two defects that move apart on either side of the line of symmetry. We present a simple theory to explain the main features of the experiments and numerical simulations.

**2:54PM R8.00003 Anomalous persistence of a pinch in a pipe**, L. MAHADEVAN, A. VAZIRI, M. DAS, Harvard University — The response of low-dimensional solid objects combines geometry and physics in unusual ways, exemplified in structures of great utility such as a tubular shell that is ubiquitous in nature and technology. Here we provide a particularly surprising consequence of this confluence of geometry and physics in tubular structures: the anomalously large persistence of a localized pinch in an elastic pipe whose effect decays very slowly as an oscillatory exponential with a persistence length that scales as  $R^{3/2}/t^{1/2}$ , diverging as the thickness of the tube vanishes. The result is more a consequence of geometry than material properties, and is thus equally applicable to carbon nanotubes and cytoskeletal microtubules as it is to aircraft fuselages and geological plates, with a number of consequences, some of which we consider.

3:06PM R8.00004 Crystalline order on the paraboloid , LUCA GIOMI, MARK BOWICK, Syracuse University — We describe an experimental and theoretical investigation of crystalline order on a two-dimensional paraboloid. In contrast to the sphere, the paraboloid exhibits both variable Gaussian curvature and a boundary. Both these features must be treated for a thorough theoretical understanding. A macroscopic model of a parabolic crystal can be obtained in the laboratory by assembling a single layer of soap bubbles on the surface of a rotating liquid, thus extending the classic work of Bragg and Nye on planar arrays of soap bubbles.

**3:18PM R8.00005 Elastic Stiffness of Grain Boundary Scars and Dislocation Dynamics**, HOMIN SHIN, MARK BOWICK, Syracuse University — We analytically calculate the stiffness of finite-length grain boundaries (scars) on a spherical crystal within the continuum elasticity theory. The scar is composed of an isolated disclination with +1 topological charge together with a finite number of dislocations. We determine the elastic free energy of a single finite-grain boundary scar by considering interacting defects, such as Disclination-Disclination (D-D), Disclination-dislocation (D-d), and dislocation-dislocation (d-d). The harmonic potential binding dislocations to the scar is obtained by determining the free energy of a single dislocation perturbed away from its equilibrium position. The elastic spring constants so obtained are compared to experimental data on dislocation dynamics [1]. We conclude with some comments on interstitial dynamics. [1] Lipowsky, P., Bowick, M. J., Meinke, J. H., Nelson, D. R. and Bausch, A. R. Nature Mater. 4, 407-411 (2005).

3:30PM R8.00006 Membrane Nano-Structures: The Three Tether Junction , OLIVER RUEBENACKER, University of Connecticut, GREG HUBER, University of Connecticut — Tethers are robust cylindrical nanostructures of lipid bilayer membranes, including biomembranes. They can be easily produced in experiments and can be found in and on cells. Tethers are useful for probing the mechanical properties of membranes, because the radius of a tether is small enough to make the bending stiffness of the membrane relevant. In an experiment, a glass bead was attached to a tether and pulled with a laser tweezer leading to the formation of a three tether junction. I will present a theory explaining the observed force-displacement relationship and simulation results of the shape of the three tether junction.

3:42PM R8.00007 Toward a multi-scale simulation of lipid bilayer systems, TAISUKE SUGII, SHU TAKAGI, YOICHIRO MATSUMOTO, The University of Tokyo — In numerical simulations of lipid bilayer systems, it has become important to treat the membrane molecules (e.g., lipids, proteins, and drug molecules) explicitly for designing medical drugs and for developing drug delivery systems. However, it is difficult to apply straightforwardly a microscopic simulation technique such as the molecular dynamics method to the large-scale bilayer systems, because the length and the time scales of these systems are very large compared to the scales of the molecules. The authors take two approaches for this problem. First, we use the dissipative particle dynamics method and the coarse grained molecular dynamics method in addition to the standard molecular dynamics method. The results are compared with the molecular-dynamics results and experimental data. Secondly we use a molecular dynamics and continuum hybrid simulation method. In this method, the region near the membrane is computed by an atomistic-simulation method and the solvent region is computed by a continuum-simulation method. (In our study, the coarse grained molecular dynamics was used for the atomistic region.) The validity and availability of this later approach will be discussed.

#### 3:54PM R8.00008 Influence of the size of interacting domains on the diffusion of nano-particles

, FLORIAN RÜCKERL, CARSTEN SELLE, JOSEF KÄS — Single particle tracking (SPT) is widely used for investigating the diffusion of proteins in cell membranes. However, short lifetime and the blinking of fluorescent tracers make it difficult to obtain sufficient data on the interactions with the inhomogeneities of the membrane. Langmuir lipid monolayers provide control over obstacle size and the corresponding interaction energy since their condensed domains within liquid phases exhibit a net dipole moment. The diffusion of a stable, negatively charged latex bead in the coexisting liquid phase, with a dipole moment anti parallel to the one of the domain, was observed by SPT. The interaction energy was obtained by Boltzmann statistics of the tracking data. The electric field of the monolayer domains varies with domain size. Its distance dependence can principally change from  $E \sim 1/r^3$  for a single dipole to  $E \sim 1/r$  for large domains (R > 10m). The influence of this change on the particle diffusion was investigated by Monte Carlo simulations. The analysis shows that the particles are stronger trapped at the domain border of smaller domains and that a change from two to one dimensional diffusion occurs. Recently, we also started analogous experiments using red blood cells and vesicles as biomembrane mimics.

#### 4:06PM R8.00009 Control of domain formation and budding in multicomponent bilayer mem-

**branes**, KURT A. SMITH, ANNA C. BALAZS, University of Pittsburgh — Phase separation in fluid bilayer membranes, of lipids or block copolymers, can lead to a budding transition when line tension between the two phases comes to dominate the bending rigidity of the membrane. This leads to a nearly spherical bud connected to the membrane by a small neck. We examine the role of molecular architecture and composition on this shape transformation. Specifically we consider the inclusion of twin-tail amphiphiles which lower the free energy of the system by segregating to the interface between the two phases. Such additives can be used to lower the surface tension, thus controlling the critical size at which buds form. In addition they stabilize the neck when budding does occur, by acting essentially as stitches, thereby increasing the energy needed to detach the bud from the membrane. Using dissipative particle dynamics we are able to simulate the dynamics of large mebrane patches over relevant time scales.

4:18PM R8.00010 Ordering by collapse: Two-dimensional crystallization of hydrophobic dimers by folding Langmuir monolayers<sup>1</sup>, DAVID VAKNIN, Ames Laboratory, Iowa State University, ALEX TRAVESSET, Ames Laboratory, Iowa State University — Synchrotron X-ray studies of arachidic-acid monolayers compressed to the collapse region, beyond their densely packed molecular area, reveal that the resulting structures are stable and exhibit a surprising degree of order. Different structures, depending on whether the monolayer is spread on pure water or on CaCl<sub>2</sub> solutions, are identified. On pure water the collapsed monolayer forms a stable crystalline trilayer, with acyl-chain packing practically identical to the 3D crystal structure of fatty acids. For monolayers spread on Ca<sup>2+</sup> solutions, the collapse regime consists of an inverted bilayer with the hydrophobic tails in contact with the water surface and the calcium ions bridging the polar heads. The inverted bilayer structure possesses a well ordered crystalline slab of calcium-oxalate-monohydrate intercalated between two acyl-chains. We discuss the implications of our findings to recent reports on dewetting of water near hydrophobic surfaces, on the formation of super-lattice structures by ions beneath a monolayer, and the relevance to certain biological processes.

<sup>1</sup>The MUCAT sector at the APS, through Ames Laboratory, and the use of the APS are supported by U.S. DOE, Basic Energy Sciences under Contracts Nos. W-7405-Eng-82 and W-31-109-Eng-38, respectively.

4:30PM R8.00011 Mechanical Properties of an Actin Filament Network Monolayer<sup>1</sup>, ROBERT WALDER, MICHAEL DENNIN, U. C. Irvine Department of Physics and Astronomy, ALEX LEVINE, UCLA Department of Chemistry and Biochemistry — Actin filament networks present a model system to study the mechanical properties of semi-rigid polymer networks. Because they are a network, the filaments can display behavior that deviates from continuum elasticity theory on sufficiently short length scales, resulting in interesting nonlinear response of the system to applied stresses and strains. We have developed a Couette (concentric cylinders) style apparatus to study monolayers of actin confined to the air-water interface. This talk will present results characterizing the response of the monolayer to continuous and step-wise strains. We will report on measurements of the viscosity of the actin network, as a macroscopic characterization, and on tracking of particles embedded in the network. The particle tracking is used to probe local displacements of the network in response to applied strain. We will report on tests of the predicted transition between affine and non-affine displacements as a function of cross-linking density.

<sup>1</sup>supported by NSF grant DMR-0354113

## 4:42PM R8.00012 Shape Selection in Self-Assembled Chiral Membranes: New Mechanism Based on the Flexoelectric Effect, ZHAO LU, ROBIN SELINGER, JONATHAN SELINGER, Liquid Crystal Institute, Kent State University — Many biological materials self-assemble into chiral microstructures such as cylindrical tubules and helical ribbons. A chiral elastic theory proposed by Selinger et al., based on the elastic properties and chirality of amphiphilic lipid molecules, has been successful in explaining the formation of tubules and helical ribbons. Recently, an experiment has shown that achiral lipid molecules can also form chiral microstructures. This challenges the previous theory based on molecular chirality. Toward understanding this problem, we develop a new model for membrane shape selection based on the flexoelectric effect. We investigate this model through both analytical calculations and dissipative particle dynamic simulations on tethered membranes.

#### 4:54PM R8.00013 Bile Salt Mediated Growth of Reverse Wormlike Micelles in Nonpolar

**Liquids**, SHIH-HUANG TUNG, YI-EN HUANG, SRINIVASA RAGHAVAN, Department of Chemical and Biomolecular Engineering, University of Maryland, College Park, MD 20742 — We report the growth of reverse wormlike micelles induced by the addition of a bile salt in trace amounts to solutions of the phospholipid, lecithin in nonpolar organic solvents. Previous recipes for reverse wormlike micelles have usually required the addition of water to induce reverse micellar growth; here, we show that bile salts, due to their unique "facially amphiphilic" structure, can play a role analogous to water and promote the longitudinal aggregation of lecithin molecules into reverse micellar chains. The formation of transient entangled networks of these reverse micelles transforms low-viscosity lecithin organosols into strongly viscoelastic fluids. The zeroshear viscosity increases by more than five orders of magnitude, and it is the molar ratio of bile salt to lecithin that controls this viscosity enhancement. The growth of reverse wormlike micelles is also confirmed by small-angle neutron scattering (SANS) experiments on these fluids.

5:06PM R8.00014 Mesoscopic simulations of binary mixtures and microemulsions using a stochastic, particle-based algorithm, ERKAN TUZEL, School of Physics and Astronomy, University of Minnesota, GUOAI PAN, THOMAS IHLE, DANIEL KROLL, Department of Physics, North Dakota State University — Particle-based simulation techniques provide an attractive alternative to traditional methods for the coarse-grained modeling of a fluctuating solvent. A particularly appealing algorithm introduced by Malevanets and Kapral[1], called Stochastic Rotation Dynamics, describes a fluid with an ideal gas equation of state. The algorithm has been successfully applied to study polymers, colloids, and vesicles in shear flow. Recently, this algorithm has been generalized to model fluids with non-ideal equations of state[2]. We will discuss how this can be used to study binary mixtures with a miscibility gap. Results for the demixing such as the phase diagram and measurements of interface fluctuations and the surface tension of a droplet will be shown. By tuning the ratio of surface tension and viscosity both damped and overdamped capillary waves were obtained. The coarsening of domains during spinodal decomposition is also investigated. In order to describe microemulsions, the model is further extended to include surfactant molecules. Preliminary results for the onset of emulsification will be presented. [1] A. Malevanets, R. Kapral, J. Chem. Phys. 110, 8605 (1999). [2] T. Ihle, E. Tuzel, D. M. Kroll, cond-mat/0509631; cond-mat/0511312.

5:18PM R8.00015 On the bouncing of rigid spheres on thin polymer films, LAURENT COURBIN, ANTONIN MARCHAND, ASHKAN VAZIRI, HOWARD A. STONE, Division of Engineering and Applied Sciences, Harvard University — We report on a study of the rebound of stainless steel spheres on thin polymer films. After the sphere is dropped it bounces off the plastic sheet and the evolution in time of the subsequent rebounds are recorded. Experiments are performed varying the sphere radius, the impact velocity, and the film tension. The variations of the contact time, the amplitude of deformation of the film, and the loss of energy of the sphere after impact, as reported via a coefficient of restitution, lead to a number of scaling relations. These results are interpreted in terms of linear and nonlinear theories of the elasticity of membranes.

## Wednesday, March 15, 2006 2:30PM - 5:18PM – Session R21 DFD DBP: Focus Session: Biological Hydrodynamics Baltimore Convention Center 318

2:30PM R21.00001 Large-scale pattern formation in active particles suspensions: from interacting microtubules to swimming bacteria<sup>1</sup>, IGOR ARANSON, Argonne National Laboratory — We consider two biological systems of active particles exhibiting large-scale collective behavior: microtubules interacting with molecular motors and hydrodynamically entrained swimming bacteria. Starting from a generic stochastic microscopic model of inelastically colliding polar rods with an anisotropic interaction kernel, we derive set of equations for the local rods concentration and orientation. Above certain critical density of rods the model exhibits orientational instability and onset of large-scale coherence. For the microtubules and molecular motors system we demonstrate that the orientational instability leads to the formation of vortices and asters seen in recent experiments. Similar approach is applied to colonies of swimming bacteria Bacillus subtilis confined in thin fluid film. The model is formulated in term of two-dimensional equations for local density and orientation of bacteria coupled to the low Reynolds number Navier-Stokes equation for the fluid flow velocity. The collective swimming of bacteria is represented by additional source term in the Navier-Stokes equation. We demonstrate that this system exhibits formation of dynamic large-scale patterns with the typical scale determined by the density of bacteria.

<sup>1</sup>This research was supported by US DOE, contract #W-31-109-ENG-38

 $3:06PM \ R21.00002 \ Elastic \ swimming \ I: \ Optimization$  , eric lauga, tony yu, anette hosoi, mit — We consider the problem of swimming at low Reynolds number by oscillating an elastic filament in a viscous liquid, as investigated by Wiggins and Goldstein (1998, Phys Rev Lett). In this first part of the study, we characterize the optimal forcing conditions of the swimming strategy and its optimal geometrical characteristics.

 $3:18\mathrm{PM}\ \mathrm{R21.00003}\ \mathrm{Elastic}\ \mathrm{swimming}\ \mathrm{II:}\ \mathrm{Experiments}$  , tony Yu, eric lauga, anette hosoi, mit — We consider the problem of swimming at low Reynolds number by oscillating an elastic filament in a viscous liquid, as investigated by Wiggins and Goldstein (1998, Phys Rev Lett). In this second part of the study, we present results of a series of experiments characterizing the performance of the propulsive mechanism.

3:30PM R21.00004 Stress-induced reversal of flagellar propulsion: an ingredient of quorum polarity of Bacillus subtilis<sup>1</sup>, L. CISNEROS, C. DOMBROWSKI, R.E. GOLDSTEIN, J.O. KESSLER, University of Arizona — Recent experiment have shown large-scale dynamic coherence in suspensions of the bacterium B. subtilis, characterized by quorum polarity – the collective parallel swimming of cells. To probe mechanisms leading to quorum polarity, we study the response of individual B. subtilis cells to steric stress brought on by swimming into a micron-sized spatial constriction. Careful visualization shows that cells can fully reverse their swimming direction at spatial constrictions without turning the cell body. This property, termed "flippancy," is quantified by measurements of the inward and outward swimming velocities, accelerations and decelerations, and docking times. The asymptotic inward and outward swimming speeds far from the constriction show near perfect correlation, implying that the propelling flagella flip, and that "forwards" and "backwards" are dynamically indistinguishable, as with E. coli. Implications for the collective dynamics are discussed.

<sup>1</sup>Supported in party by NSF Grant PHY-0551742

3:42PM R21.00005 Effects of nonlinear membrane elasticity on capsule recovery<sup>1</sup>, and respectively <math>3:42PM R21.00005 EffectsGONZALEZ-MANCERA, CHARLES EGGLETON, UMBC — The recovery of a capsule from an initially deformed shape is considered. The problem is solved numerically for a capsule made of an incompressible liquid surrounded by a thin elastic membrane using the Boundary Integral Method. Elastic membranes with different constitutive models providing a wide range of behaviors at large deformations (strain-hardening, strain- softening and linear elastic) were considered. The results suggest that the recovery process is dominated by the isotropic dilatation modulus. The recovery process from small deformations was seen to be nearly independent of the membrane constitutive model. Recovery from large deformations was highly dependent on the constitutive model and the initial geometry of the capsule. Analysis of the recovery from large deformations demonstrated that the process is modulated by the tangential component of the elastic traction, \Ft, acting on the membrane. This component of the traction was seen to either favor or oppose the recovery depending on the constitutive equation used to model the elastic membrane. The differences in the recovery process can be used to identify the best model for a particular capsule based on features observed during the recovery process.

<sup>1</sup>supported by NIH/NIAID RO1AIO63366

#### 3:54PM R21.00006 Balancing energy input and viscous dissipation in the Zooming

**BioNematic**<sup>1</sup>, J.O. KESSLER, U. Arizona, R.E. GOLDSTEIN, University of Arizona, R. CORTEZ, Tulane U. — Beyond a concentration threshold, populations of the swimming bacteria *Bacillus subtilis* form a phase (the Zooming BioNematic=ZBN) comprising intermittent domains of co-aligned cells all swimming in the same direction. Collectively generated hydrodynamic forces between bacteria, the cells' ability to flip flagella, thereby changing swimming polarity, and their tendency to swim upstream into a collectively generated current are fundamental interactions leading to the ZBN. But how does the ZBN generate dynamic patterns, similar to ones at  $Re \gg 1$ ? The energy put into the fluid by the swimming organisms overwhelms viscous damping, as demonstrated by a new dimensionless ratio Bs, analogous to Re but replacing the numerator by a measure of bacterial energy input. The magnitude of Bs is estimated via the Navier-Stokes equations, considering individual bacteria at moderate concentration, and entire domains at high. Bs is proportional to the bacterial concentration, Bs is independent of viscosity.

<sup>1</sup>Supported in part by NSF grants PHY-05541742 and DEB-0075296

#### 4:06PM R21.00007 Multicellularity and the Functional Interdependence of Motility and Mole-

**cular Transport**<sup>1</sup>, C. SOLARI, S. GANGULY, J.O. KESSLER, R. MICHOD, R.E. GOLDSTEIN, U. of Arizona — Benefits, costs and requirements accompany the transition from motile totipotent unicellular organisms to multicellular organisms having cells specialized into reproductive (germ) and vegetative (sterile soma) functions such as motility. In flagellated colonial organisms such as the volvocalean green algae, organized beating by the somatic cells' flagella yields propulsion important in phototaxis and chemotaxis. It has not been generally appreciated that for the larger colonies, flagellar stirring of boundary layers and remote transport are fundamental for maintaining a sufficient rate of metabolite turnover, one not attainable by diffusive transport alone. We describe experiments that quantify the role of advective dynamics in enhancing productivity in germ-soma differentiated colonies. First, experiments with suspended deflagellated colonies of *Volvox carteri* show that forced advection improves productivity. Second, Particle Imaging Velocimetry of fluid motion around colonies reveals flow fields with very large characteristic velocities U extending to length scales comparable to the colony radius R. For a typical metabolite diffusion constant D, the Peclet number  $Pe = 2UR/D \gg 1$ , indicative of the dominance of advection over diffusion, with striking augmentation at the cell division stage.

<sup>1</sup>Supported in part by NSF grants DEB-0075296 and PHY-0551742

4:18PM R21.00008 Flagella-Driven Flows Circumvent Diffusive Bottlenecks that Inhibit Metabolite Exchange<sup>1</sup>, MARTIN SHORT, CRISTIAN SOLARI, SUJOY GANGULY, JOHN KESSLER, RAYMOND GOLDSTEIN, University of Arizona, THOMAS POWERS, Brown University — The evolution of single cells to large and multicellular organisms requires matching the organisms' needs to the rate of exchange of metabolites with the environment. This logistic problem can be a severe constraint on development. For organisms with a body plan that approximates a spherical shell, such as colonies of the volvocine green algae, the required current of metabolites grows quadratically with colony radius whereas the rate at which diffusion can exchange metabolites grows only linearly with radius. Hence, there is a bottleneck radius beyond which the diffusive current cannot keep up with metabolic demands. Using *Volvox carteri* as a model organism, we examine experimentally and theoretically the role that advection of fluid by surface-mounted flagella plays in enhancing nutrient uptake. We show that fluid flow driven by the coordinated beating of flagella produces a convective boundary layer in the concentration of a diffusing solute which in turn renders the metabolite exchange rate quadratic in the colony radius. This enhanced transport circumvents the diffusive bottleneck, allowing increase in size and thus evolutionary transitions to multicellularity in the Volvocales.

<sup>1</sup>Supported by NSF Grants DEB-0075296, PHY-0551742 and CMS-0093658

#### 4:30PM R21.00009 Measurement of Flow Patterns and Dispersion in the Human Airways<sup>1</sup>,

FRANK E. FRESCONI, AJAY K. PRASAD, Department of Mechanical Engineering, University of Delaware — A detailed knowledge of the flow and dispersion within the human respiratory tract is desirable for numerous reasons. Both risk assessments of exposure to toxic particles in the environment and the design of medical delivery systems targeting both lung-specific conditions (asthma, cystic fibrosis, and chronic obstructive pulmonary disease (COPD)) and system-wide ailments (diabetes, cancer, hormone replacement) would profit from such an understanding. The present work features experimental efforts aimed at elucidating the fluid mechanics of the lung. Particle image velocimetry (PIV) and laser induced fluorescence (LIF) measurements of oscillatory flows were undertaken in anatomically accurate models (single and multi-generational) of the conductive region of the lung. PIV results captured primary and secondary velocity fields. LIF was used to determine the amount of convective dispersion across an individual generation of the lung.

<sup>1</sup>Sponsored by Philip Morris USA Inc. and Philip Morris International

 $4:42PM\ R21.00010\ On\ small\ insect\ flight\ -\ a\ two-dimensional\ study$ , PAULO FERREIRA DE SOUSA, New Mexico State University — Small insect\ flight\ is\ characterized\ by\ very\ small\ Reynolds\ numbers\ and\ relatively\ simple\ wing\ motions. In this\ study,\ a\ two-dimensional\ approximation\ of\ small\ insect\ flight\ is\ characterized\ by\ very\ small\ Reynolds\ numbers\ and\ relatively\ simple\ wing\ motions. In this\ study,\ a\ two-dimensional\ approximation\ of\ small\ insect\ flight\ is\ characterized\ by\ very\ small\ Reynolds\ numbers\ and\ relatively\ simple\ wing\ motions. In this\ study,\ a\ two-dimensional\ approximation\ of\ small\ insect\ flight\ is\ characterized\ by\ very\ small\ Reynolds\ numbers\ and\ relatively\ simple\ wing\ motions. In this\ study,\ a\ two-dimensional\ approximation\ of\ the\ motion\ of\ the\ flight\ of\ Drosophila\ melanogaster,\ and\ was\ done\ in\ line\ with\ previous\ experimental\ and\ numerical\ simulations\ available\ in the\ literature. Calculations\ were\ carried\ out\ until a\ time-periodic\ steady-state\ was\ achieved. Changes\ in\ lift\ generation\ and\ vortex\ dynamics\ are\ studied\ for\ Reynolds\ numbers\ spanning\ two\ orders\ of\ magnitude,\ in\ order\ to\ accurately\ find\ the\ critical\ Re\ number,\ vortices\ are\ alternately\ shed\ during\ translation. Below\ the\ critical\ Reynolds\ number,\ vortices\ are\ formed\ during\ translation,\ creating\ two\ articles\ are\ flow\ the\ critical\ Reynolds\ number,\ vortices\ are\ alternately\ shed\ during\ translation. Below\ the\ critical\ Reynolds\ number,\ vortices\ are\ flow\ the\ critical\ Reynolds\ number,\ vortices\ are\ alternately\ shed\ during\ translation\ significant\ because,\ below\ it,\ an\ important\ mechanism\ of\ lift\ generation\ no\ lift\ seconds\ seconds\ number,\ vortices\ are\ flow\ the\ critical\ Reynolds\ number,\ vortices\ are\ flow\ shed\ during\ translation\ seconds\ seco

4:54PM R21.00011 Wake characteristics of a model ornithopter , ALFREDO JUAREZ, New Mexico State University, JACOB HARLOW, New Mexico State University, JAMES ALLEN, New Mexico State University, PAULO FERREIRA DE SOUSA — This paper details unsteady wake measurements from a model Ornithopther flying in a wind tunnel at representative flight conditions. Testing over a range of Strouhal number, 0.1-0.3, shows that the unsteady wake is composed of coherent vortical structures that resemble vortex rings. A single ring is formed in the wake of each wing during one wing beat. Momentum balance from velocity field measurements are reconciled with unsteady lift and drag measurements from a drag balance.

5:06PM R21.00012 Vertical hovering of a symmetric flapping model, MAKOTO IIMA, TATSUO YANAGITA, Hokkaido University — We study the motion of a model equipped with flapping wings under the influence of gravity (external force). This model moves in a two-dimensional fluid according to the hydrodynamic force generated by vortices separated from its wings. As a result of the interaction between the vortices and the wings, the model moves steadily in a direction against the gravity. Moreover, hovering, i.e., a steady flight staying in a particular position, can be achieved here by the effective use of vortex structures enhancing the hydrodynamic force that supports the model against gravity. The system exhibits a transition from the state with hovering to a state where hovering is impossible, as the model parameters are changed.

#### Wednesday, March 15, 2006 2:30 PM - 5:30 PM -

Session R34 DFD: Turbulence Baltimore Convention Center 337

2:30PM R34.00001 Measurements of the Multifractal Dimension of Lagrangian Turbulence<sup>1</sup>, NICHOLAS OUELLETTE, HAITAO XU, Cornell University, EBERHARD BODENSCHATZ, Cornell University and Max Planck Institute for Dynamics and Self-Organization — We report experimental measurements of the Lagrangian multifractal dimension spectrum in an intensely turbulent laboratory water flow by the optical tracking of tracer particles. These measurements are compared with three model dimension spectra. The Legendre transform of the measurements is found.

<sup>1</sup>This work was supported by the NSF and by the Max Planck Society.

#### 2:42PM R34.00002 Multifractal particle distribution in compressible turbulence on a free

 $surface.^1$ , WALTER GOLDBURG, MAHESH BANDI, Department of Physics and Astronomy, University of Pittsburgh, JOHN CRESSMAN, Krasnow Institute, George Mason University — The distribution of particles in compressible turbulence on a free surface is inhomogeneous. The floaters flee regions of fluid up-wellings and cluster into ridge-like structures near fluid down-wellings. The concentration of floaters is measured on the surface of a large tank of turbulently stirred water. The multifractal structure of the clusters is reflected in the moments of particle concentration. The results are compared with recent work of Bec *et.al.* [J. Bec, K. Gawedzki and P. Horvai, Phys. Rev. Lett., 92, 224501 (2004)] conducted on synthetic velocity fields that follow the compressible Kraichnan model.

<sup>1</sup>This work is supported by the NSF under Grant No. DMR-0201805.

2:54PM R34.00003 Velocity and Scalar intermittency in restricted Euler dynamics , YI LI, CHARLES MENEVEAU, Johns Hopkins University — A long standing problem in turbulence is to predict the intermittency from Navier-Stokes equation. Recently, by adopting a Lagrangian point of view and using the restricted Euler dynamics, we derived a simple nonlinear dynamical system, called advected delta-vee system, for the time evolution of longitudinal and transverse velocity increments, from which we showed that the non-Gaussian tails in turbulence originate from the inherent self-amplification of longitudinal velocity increments, and cross amplification of transverse velocity increments. Here, after reviewing previous results, the analysis is generalized to the increments of a passive scalar. A simple nonlinear equation is derived for the time evolution of scalar increments. The equation is coupled to the advected delta-vee system through the squeezing effect of the longitudinal velocity increments, suggesting the system captures important trends in the original Navier-Stokes and scalar transport dynamics.

#### 3:06PM R34.00004 How Gaussian is the Velocity Gradient Tensor at Large Scales in Hydrody-

**namic Turbulence?**, LAURENT CHEVILLARD, YI LI, CHARLES MENEVEAU, The Johns Hopkins University, Baltimore, MD. — Fully developed turbulent flows exhibit a continuous range of exited scales, from the finest (dissipative range) towards the integral scale where energy is injected. Many theoretical approaches use the assumption that at large scales the fluctuations display Gaussian statistics. This has also been repeatedly confirmed based on measurements of longitudinal velocity increments in the Eulerian framework and temporal velocity increments in the Lagrangian framework. When the separation is comparable to integral scales of the flow, the PDFs of these velocity increments display Gaussian statistics, in contrast to the elongated tails and non-Gaussian statistics at smaller scales. Motivated by recent insights gained from Restricted Euler dynamics, we examine the statistics of the full velocity gradient tensor and several of its invariants relevant to the transfer of energy from large to small scales. Using Direct Numerical Simulations, we study the coarse-grained and band-pass Eulerian velocity gradient tensor. Among other features, we show that even at the integral length scale, the gradient statistics deviate from Gaussianity.

3:18PM R34.00005 Quantum Fluid Mechanical Theory of Turbulence, DAVID DROSDOFF, ALLAN WIDOM, Northeastern University, YOGENDRA SRIVASTAVA, Northeastern University, INFN, University of Perugia — Turbulence has been called the last great unsolved problem of classical physics. The difficulty of solving the turbulence problem classically (even with the help of recent large scale computer simulations) may be that the problem is not classical. Turbulence will here be described as due to the non-commuting nature of the components of the Landau quantum fluid velocity field. The formation of fractal dimensional regions of quantum vortex strings in fully developed turbulence will be discussed along with the implied Kolmogorov scaling functions.

3:30PM R34.00006 Counter-gradient transport in the atmospheric boundary layer , CHERYL KLIPP, US Army Research Laboratory — Counter-gradient transport in turbulent flows, also called negative viscosity, has been theorized and observed over the past century at a variety of spatial scales. More than one mechanism may be responsible for the process of transferring momentum from slower moving fluid to faster moving fluid depending on the scale of the flow and other flow properties. Horizontal divergence is presented as a possible mechanism for counter-gradient momentum transport observed in the atmospheric boundary layer.

3:42PM R34.00007 LES Simulations of Pulsed Gas Jets. , JONATHAN ANDERS, Purdue University, VINICIO MAGI, Purdue University, JOHN ABRAHAM, Purdue University — The study of pulsed jets is motivated by their applications which include increasing mixing, enhancing heat transfer, and controlling flow separation and vortex structures. This work investigates the interaction between gas jet pulses in the near-field using large eddy simulation (LES). LES employing the constant coefficient Smagorinsky model is compared to Reynolds-averaged Navier-Stokes (RANS) simulations with a two-equation  $k \in model$ . RANS predictions indicate faster penetration of subsequent jet pulses caused by the mean flow field from the first pulse, and do not show enhanced mixing due to residual turbulence. LES of the jet near-field includes development of the head vortex ring and transition to turbulence in the jet. LES of the pulsed gas jet predicts interaction of the head vortex with residual turbulence from an earlier pulse. The dominant effect of the mean flow field and the accelerated penetration seen in RANS predictions are not evident in the LES results.

3:54PM R34.00008 Vortical structures in a flume, R. GURKA, Dept. of Mech. and Mat. Engr., Univ. of Western Ontario, A. LIBERZON, Inst. of Hydromechanics and Water Resources Mgmt., ETH Zurich, Switzerland, G. HETSRONI, Faculty of Mech. Engr., Technion, Israel — We report the results of statistical spatial characterization of coherent structures in turbulent boundary layer in a flume. The characterization approach is based on the proper orthogonal decomposition (POD) of vorticity, elucidating large-scale coherent patterns in a turbulent boundary layer. The method was successfully applied to the two- and three-dimensional experimental data extracted from particle image velocimetry (PIV), and multi-plane stereoscopic PIV (XPIV) respectively, and the three-dimensional data from direct numerical simulation (DNS) in a channel flow. The large-scale structure was obtained by using linear combination of POD eigenmodes of vorticity. POD allows for methodological analysis of the properties of the educed structure in the different measurement planes (orthogonal in the case of 2D PIV and parallel in the case of XPIV) and in the different cross-sections of the DNS data. Based on the statistical approach we suggest a conceptual model of large-scale coherent structures in a turbulent boundary layer flow that incorporates the experimental and the numerical results. The proposed conceptual model is a spiral vortical structure attached to the wall and expanding in both the spanwise and the wall-normal directions. Its shape resembles a funnel structure and a 'double-cone eddy' concept. The relationship of the model to the structures in the near wall region is presented.

4:06PM R34.00009 Single-point Velocity Statistics , YONGGUN JUN, X.L. WU, University of Pittsburgh — The singlepoint (SP) velocity statistics is investigated in forced and decaying two-dimensional turbulence in a flowing soap film. It is shown that the probability distributin functions (PDF) in both cases deviate from a Gaussian distribution, which is normally anticipated in turbulent fluid flows. In the forced turbulence case, the tail of the SP velcoty PDF decays faster than Gaussian and can be correlated with the forcing statistics on small sclaes. In the decaying turbulence case, the SP velocity PDF evolves from a sub-Gaussion to a super- Gaussian behavior as a function of decaying time. In all times, however, the locally averaged vorticity distribution remains approximately Gaussian. While our forcing data may be explained by the instanton model put forward by Falkovich et al., the decaying turbulence data remain unexplained by theory.

4:18PM R34.00010 Coherent Structures in Decaying Two-Dimensional Turbulence , MICHAEL RIVERA, Los Alamos National Laboratory, MICHAEL TWARDOS, ROBERT ECKE — We revisit the matter of coherent structures, such as vortices, and their role in decaying two-dimensional turbulence. These experiments take place in an electromagnetically forced stratified layer within a square container with no slip boundaries and a linear dissipation with the container bottom. Results relating the energy and enstrophy of the bulk flow with the number and strength of coherent vortices are compared with earlier numerical and experimental work.

4:30PM R34.00011 Multiscale Distribution of Energy Transfer in Two Dimensional Turbulence , MICHAEL TWARDOS, MICHAEL RIVERA, ROBERT ECKE — In two dimensional turbulence, the mechanisms responsible for energy transfer to larger scales are not well understood. We present results from an experimental system consisting of a square meter of electromagnetically driven thin salt water layer that is used to investigate this inverse energy cascade. A filter technique applied to high resolution velocity fields is used to understand scale to scale energy transfer. An extension of this technique determines the contribution of energy transfer across a given length scale from smaller scales. Expanding the subgrid coupling terms allows for some speculation of the energy transfer mechanisms.

4:42PM R34.00012 Statistical Properties of 2 Dimensional Turbulence in a Finite Box, COLM CONNAUGHTON, Center for Nonlinear Studies, Los Alamos National Laboratory, MISHA CHERTKOV, Theoretical Division, Los Alamos National Laboratory, VLADIMIR LEBEDEV, Landau Institute for Theoretical Physics, IGOR KOLOKOLOV, Landau Institute for Theoretical Physics — In the standard statistical theory of two dimensional hydrodynamics forced at some intermiediate scale, two cascades are produced. Energy flows to large scales, producing Kolmogorov's  $k^{-5/3}$  spectrum at small k and enstrophy flows to small scales to produce Kraichnan's  $k^{-3}$  spectrum at large k. If we consider turbulence in a finite box in the absence of large scale dissipation, the inverse cascade eventually reaches the size of the box and the cascade is blocked. This leads to accumulation of energy in the largest modes, a process which can be qualitatively thought of as a nonequilibrium condensation process. The "condensate" in this case is a coherent, large scale vortex dipole. We investigate how the system passes through a series of distinct regimes, leading to the emergence of this large scale structure. We show how it affects the scaling properties of two-dimensional turbulence and explain how the presence of very strong vortices leads to an apparent modification of the small scale statistical properties of the inverse cascade.

4:54PM R34.00013 Direct Numerical Simulations of Turbulent Flow in a Wavy Channel, LUO WANG, KOSTAS HOUSIADAS, ANTONY BERIS, University of Delaware — A spectrally preconditioned biconjugate gradient algorithm (Bi-CGSTAB) has been developed that enabled us to perform high accuracy (spectral) efficient Direct Numerical Simulations (DNS) of Newtonian turbulent flow in an undulating channel geometry. The DNS of have been performed in a channel geometry involving a single sinusoidal solid wavy wall with amplitude/half width ratio of 0.1 and a wave length of 2. Two different friction Reynolds numbers have been investigated, Re<sub>7</sub>=160 and 220 corresponding to mean Reynolds numbers (based on the channel half width) 1800 and 2480, respectively. The computational domain used was 10x2x5 along the streamwise, shearwise and spanwise direction respectively, with spectral resolutions ranging from 160x257x64 to 320x385x128. The numerical results compare well against Hudson's measurements (Hudson, Ph.D. Thesis, UIUC 1993). In addition, the DNS results allowed us to investigate in detail various turbulence statistics and the vorticity structure and its influence from the wall undulation.

5:06PM R34.00014 Non-Boussinesq effects on heat transport in turbulent Rayleigh-Bénard convection of gases<sup>1</sup>, DENIS FUNFSCHILLING, UCSB, GUENTER AHLERS, UCSB — In turbulent Rayleigh-Bénard convection large temperature differences often are used in order to reach very high Rayleigh numbers. This can lead to a breakdown of the Boussinesq approximation which assumes temperature-independent fluid properties. We presents quantitative measurements of non-Boussinesq (NB) effects on the heat transport obtained by using Ethane gas at a mean temperature of 40°C and pressures up to 40 bars. At the largest temperature differences of about 40°C, where the top of the sample approached the vapor-liquid saturation curve, the Nusselt number was increased above the Boussinesq value by several percent. This contrasts with NB effects in liquids<sup>2</sup> where the heat transport is reduced below the Boussinesq value.

<sup>1</sup>Supported by DOE Grant DE-FG02-03ER46080

<sup>2</sup>G. Ahlers, E. Brown, D. Funfschilling, S. Grossmann, and D. Lohse, J. Fluid Mech., submitted.

#### 5:18PM R34.00015 Lattice Boltzmann studies of drag reduction in turbulent channel flow

with polymers., ALEXANDER KARPIKOV, Yale University, S.A. ORSZAG, K.R. SREENIVASAN — Massive drag reduction in turbulent flow by dilute addition of polymers has long been a challenging problem in fluid dynamics. In order to study this problem here we use the Lattice Boltzmann method (LBM) to simulate turbulent channel flow. A polymer model, which is macroscopically equivalent to the FENE-P model, is included in LBM to represent polymers. Drag reduction with polymers was observed in the simulations. Although such drag reduction has been demonstrated in laboratory experiments, the mechanisms are not yet clear. In order to understand these results we investigated the role of dilute polymers on Kelvin-Helmholtz instability in the much simpler turbulent mixing layer. Our simulations of the mixing layer show that polymers produce a stabilizing effect and suppress momentum transport due to fluctuating velocity components. The simulations of these two systems together provide a clearer picture of the interaction between polymers and coherent structures in the near-wall region of the turbulent flow and shed light on the mechanism of drag reduction. The addition of polymers primarily modifies turbulent bursts in channel flow, and this phenomenon has several features in common with the effect of polymers on Kelvin-Helmholtz instability in the mixing layer.

#### Thursday, March 16, 2006 8:00AM - 11:00AM -Session U8 DFD: Granular Materials Baltimore Convention Center 314

 $\begin{array}{l} \textbf{8:00AM U8.00001 Statistical and dynamical properties of a vibrated granular polymer}, \\ \textbf{ARSHAD} \\ \textbf{KUDROLLI, MICAH VEILLEUX, Physics Dept., Clark University, MEHRAN KARDAR, Physics Dept., MIT — We investigate the structure and dynamics of granular polymers on a vibrated bed to test the applicability of models of self-avoiding random walks. The granular polymer is composed of a chain of hollow 3 mm steel beads connected by flexible links, and moves on a 30 cm diameter flat circular bed which is roughened by gluing a layer of 1 mm steel beads in order \\ \textbf{MIT} = \textbf{MIT} + \textbf{MIT} +$ to give the chain random kicks in the vertical and horizontal directions. High speed digital imaging is used to track the position of the particles to a fraction of the bead diameter using a centroid technique. Using the identified bead positions, we analyze the motion of the center of mass over a time interval  $\Delta t$ , and its standard deviation as a function of chain length L. The standard deviation is consistent with a scaling of  $\sqrt{\Delta t/L}$ . The chain end-to-end distance scales as  $L^{\nu}$ , with  $\nu \approx 3/4$  as for self-avoiding walks. The evolution of the scattering functions and the effect of the size of the container on the observed scaling will be also discussed.

time-varying forces at the bottom surface of a granular system sheared at the top. The shear is applied by rotating a roughened piston while maintaining a constant, uniaxial compressive force. We report on the force autocorrelation and the corresponding power spectrum S of the variation of force on individual grains at the bottom surface. These forces are obtained from video tracking of imprints in a pressure-sensitive birefringent layer across the bottom surface. Averaging over concentric annuli we find power-law behavior  $S \sim 1/f^{\alpha}$  over several orders of magnitude in each annulus. The power law exponents  $\alpha$  appear to be correlated with the in-plane shear strain rate. In our system friction with the stationary side walls introduces a radial gradient in the shear rate, which is maximum at the outer edge and zero at the center. The corresponding power law exponents suggest strict 1/f noise ( $\alpha = 1$ ) at the outer, shearing edge and an increasing index as one approaches the center and the shear rate vanishes.

#### 8:24AM U8.00003 Self-diffusion of particles in gas-driven granular layers with periodic flow

modulation<sup>1</sup>, CARLOS ORELLANA, Departamento de Fisica, Universidad de Chile, Santiago, Chile, IGOR ARANSON, WAI KWOK, Argonne National Laboratory, SERGIO RICA, Departamento de Fisica, Universidad de Chile, Santiago, Chile — We study particles self-diffusion in gas-driven granular layers by high-speed fluorescent video-microscopy. We show that periodic flow modulation results in an enhancement of the particle's diffusion. The diffusion enhancement, which in turn is an indication of more efficient fluidization of the granular layer, is associated with the onset of disordered sub-harmonic patterns. Our measurements provide a sensitive characterization method of the fluidization properties of particulate/gas systems.

<sup>1</sup>This research was supported by US DOE, contract #W-31-109-ENG-38.

8:36AM U8.00004 Free cooling of the one-dimensional wet granular gas, vasily zaburdaev, martin BRINKMANN, STEPHAN HERMINGHAUS, Max Planck Institute for Dynamics and Self-Organization — In the present work we consider a one-dimensional gas of hard balls covered with a thin liquid film. A liquid bridge, formed at each collision, is responsible for the hysteretic and dissipative interaction. Each rupture of a liquid bridge requires a fixed amount of energy, and thus determines a threshold of relative velocities below which the two colliding particles form a bounded state loosing their relative kinetic energy. We aim to study the cluster formation process in the free cooling system. Macroscopic laws of energy dissipation and cluster growth are studied in this model on the basis of numerical simulations supported by a scaling-like system of equations. We show that the sticky gas regime is an attracting asymptotic limit of the wet granular gas and does not dependent on the liquid bridges strength. The next neighbor velocities correlations play the key role in the establishing of this regime.

8:48AM U8.00005 A Theory of Stochastic Plasticity in Dense Granular Flow, KEN KAMRIN, MARTIN BAZANT, MIT — There have been many attempts to derive continuum models for dense granular flow, but a general theory is still lacking, which can describe different flow conditions, such as gravity-driven silo drainage and forced shear cells. Here, we start with Mohr-Coulomb plasticity for quasi-2d granular materials to calculate stresses and slip planes, but we propose a simple "stochastic flow rule" to replace the principle of co-axiality in classical plasticity. This formulation takes into account two crucial features of granular materials – discreteness and randomness at the scale of a continuum element – via diffusing "spots" which cause chain-like cooperative particle displacements, as in recent simulations of silo drainage. We postulate that spots perform random walks along slip lines, biased by body forces (gravity) and local fluidization (switch from static to dynamic friction). Stochastic plasticity allows a natural description of dense granular flows in silos and shear cells within a single theory, rooted in classical mechanics.

9:00AM U8.00006 The Solitary Wave Collision Problem in Granular Alignments<sup>1</sup>, Edgar Avalos, SUNY-Buffalo, SURAJIT SEN, SUNY-Buffalo, JAN PFANNES, Univ of Wuerzburg, T.R. KRISHNA MOHAN, SUNY-Buffalo - Any impulse travels as a solitary wave in an alignment of spherical elastic grains where the system grains are barely in contact. These solitary waves are about 7 grain diameters wide. Their speeds depend upon the maximum displacement amplitudes associated with these waves. We focus on the dynamical problem associated with the collision of two identical and opposite propagating solitary waves. Interface and grain center collisions reveal markedly different dynamics. Solitary wave collisions lead to the destruction of the original waves and the subsequent creation of new smaller waves along with "baby" or secondary solitary waves. In the absence of dissipation, these granular systems point towards the existence of a generalized equilibrium phase that involves Maxwellian distribution of velocities with no depedence on initial conditions but one that violates the equipartition theorem.

<sup>1</sup>Supported in part by NSF, ARO

#### 9:12AM U8.00007 Toward Zero Surface Tension Limit: Granular Fingering Instability in a Radial Hele-Shaw Cell, XIANG CHENG, LEI XU, AARON PATTERSON, HEINRICH JAEGER, SIDNEY NAGEL, The James Franck Institute and Department of Physics, The University of Chicago — Because of the absence of cohesive forces between grains, dry granular material can, in many respects, be thought of as a fluid with zero surface tension. In the zero surface-tension limit, viscous fingering is known to possess singular behavior. We have studied the viscous fingering instability in such a granular "fluid." In our experiment, we use a conventional radial Hele-Shaw cell consisting of two parallel glass plates separated by a gap. Gas with controlled pressures is blown through a hole at the center of one glass plate and displaces the surrounding dry granular material. We have systematically studied the fingering pattern as a function of gas pressure, gap thickness, and grain size. Two stages are observed during pattern growth.

In the first stage, we find fluid-like fingering. However, as opposed to normal fluids, the pattern is more ramified at low pressure. In the second stage, we find

several new behaviors in the system such as merging and pinching off of fingers and the existence of satellite bubbles.

9:24AM U8.00008 Force fluctuations in collisional and frictional granular flows, EMILY GARDEL, EFROSYNI SEITARIDOU, ELLEN KEENE, NALINI EASWAR, Smith College, Northampton, MA., NARAYANAN MENON, University of Massachusetts, Amherst, MA. — We make measurements of the force delivered to the wall in 2D and 3D flow geometries to explore the difference between collisional and frictional flows, and between flow geometries with and without velocity gradients in the flow direction. The distribution of force fluctuations has an exponential tail at large force in collisional flows, but falls off slower than an exponential in frictional flows. We do not see a clear signature in the force distribution of the approach to jamming and therefore the connection to force distributions in quasistatic flows remains to be understood. However, the temporal characteristics of the force fluctuations do show the approach to jamming. As reported earlier, the distribution of collision times tends to a power law in collisional flows. Similarly, the power spectrum of forces in frictional flows develops power-law behaviour at low frequencies as jamming is approached. Supported by NSF DMR 0305396 and NSF MRSEC DMR 0213695

9:36AM U8.00009 Thermal collapse of a granular gas under gravity<sup>1</sup>, LEV S. TSIMRING, University of California at San Diego, DMITRI VOLFSON, University of California at San Diego, BARUCH MEERSON, Hebrew University of Jerusalem — Free cooling of a gas of inelastically colliding hard spheres is a central paradigm of the kinetic theory of granular gases. At zero gravity the temperature of a freely cooling homogeneous granular gas follows a power law in time. How does gravity affect the cooling? We consider a semi-infinite layer of granular gas bounded from below by an elastic wall. An initially isothermal dilute granular gas is prepared in the state of hydrostatic equilibrium with barometric density distribution. We combine molecular dynamics simulations, a numerical solution of granular hydrodynamic equations and an analytic theory to show that the cooling gas undergoes thermal collapse: it condenses on the bottom of the container and cools down to zero temperature in a finite time  $t_c$  as  $T \sim (t_c - t)^2$ . The cooling scenraio is determined by the interplay between the collisional energy loss and heat conduction, while the collapse time  $t_c$  is much longer than the typical free fall time of the grains if the inelasticity of the particle collisions is small. The hydrodynamic description is found to be in excellent agreement with molecular dynamics simulations until very close to  $t_c$ .

<sup>1</sup>Support of the U.S. Department of Energy (Grant DE-FG02-04ER46135) and Israel Science Foundation is gratefully acknowledged

9:48AM U8.00010 Two particle contact lifetime distribution in gravity driven granular flow<sup>1</sup>, ROBERT BREWSTER, UCLA, LEONARDO SILBERT, University of Chicago, GARY GREST, Sandia National Laboratories, ALEX LEVINE, UCLA — The distribution of two particle contact life times for gravity driven granular flow down an inclined plane are determined from large-scale, three-dimensional discrete element simulations. Results are presented for both cohesive and non-cohesive particles for Hertzian and Hookean contact forces. The distribution of lifetimes is analyzed as a function of height from the surface for different strength  $k_n$  of the normal force, coefficient of restitution  $e_n$  and coefficient of friction  $\mu$ . In addition a generalized form of the Bagnold constitutive relation in which the shear stress depends on a sum of terms that are linear and quadratic in the shear rate is proposed for cohesive granular flows. The linear term represents a new mode of momentum transport made possible through the long lived contacts in the network while the quadratic term represents the usual Bagnold contribution from short time scale collisions. For non-cohesive grains, the strength of the linear term disappears as strength of the normal interaction  $k_n$  increased.

<sup>1</sup> Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

10:00AM U8.00011 Particle collisions in a granular  $gas^1$ , HONG-QIANG WANG, KLEBERT FEITOSA, NARAYANAN MENON, University of Massachusetts — We report a study of particle collisions in a 2D granular system vibrated in a vertical plane. We have previously studied this experimental system in a variety of contexts. With improved image analysis algorithms, we are able to locate particles with enough precision to allow detailed tracking of the collision process, when the particles are close to each other. This allows us to better study the role of the vertical walls in the collision process and to place a limit on the dissipation by mechanisms other than inelastic collisions. We report the distribution of collision parameters and comment on violations of molecular chaos resulting from the inelasticity of the system.

<sup>1</sup>We acknowledge support from NSF-DMR 0305396

**10:12AM U8.00012 Boltzmann's** *stosszahlansatz* generalized for granular contact forces , PHILIP METZGER, NASA, John F. Kennedy Space Center — Is there a valid way to generalize Boltzmann's *stosszahlansatz* (molecular chaos), the assumption that colliding molecules are not statistically correlated before the collision takes place, to the case of granular contact forces in a static packing? In thermal statistical mechanics the assumption produces a transport equation that obtains the density of single particle states and the Maxwell Boltzmann distribution. The problem in generalizing this to granular contact forces is that we must maintain the spatial symmetries of granular packing ensembles, which is not trivial. The essential trick is to sum the density of states over all particle exchanges, which destroys multi particle state information but maintains the distribution of single particle states. This summation transforms the equations into a generalized form of boson statistics. I will show that, in the summation, the first shell approximation of the fabric is transformed into the properly symmetric version of Boltzmann's *stosszahlansatz*. This produces a transport equation that obtains the density of stoses and hence the distribution of granular contact forces. Granular simulation data will also be presented to validate the theory.

#### 10:24AM U8.00013 Dynamical Heterogeneity close to the Jamming Transition in a Sheared

**Granular Material**, OLIVIER DAUCHOT, CEA/SPEC, GUILLAUME MARTY, City College of New York, GIULIO BIROLI, CEA/SPhT — The dynamics of a bi-dimensional dense granular packing under cyclic shear is experimentally investigated close to the jamming transition. Measurement of multi-point correlation functions are produced. The self-intermediate scattering function, displaying slower than exponential relaxation, suggests dynamic heterogeneity. Further analysis of four point correlation functions reveal that the grain relaxations are strongly correlated and spatially heterogeneous, especially at the time scale of the collective rearrangements. Finally, a dynamical correlation length is extracted from spatio-temporal pattern of mobility. Our experimental results open the way to a systematic study of dynamic correlation functions in granular materials.

10:36AM U8.00014 The Decorated Tapered Chain as a Granular Shock Absorber<sup>1</sup>, ROBERT DONEY, US Army Research Lab - APG, SURAJIT SEN, SUNY-Buffalo, DORIAN DICOCCO, SUNY-Buffalo — A 1D alignment of progressively shrinking spherical grains (a tapered chain) turns out to be an excellent impulse absorber with rich nonlinear dynamical behavior. Here we discuss a tapered chain with interstitial grains between every sphere of the original tapered chain and demonstrate analytically (using the hard sphere approximation), numerically and experimentally that the shock absorption ability of the "decorated" system is far superior to that of the system without the interstitial grains.

<sup>1</sup>Supported by ARO

10:48AM U8.00015 Shock Absorption by Small, Scalable, Tapered Granular Chains<sup>1</sup>, JAN PFANNES, University of Wuerzburg, ADAM SOKOLOW, Duke University, ROBERT DONEY, US Army Research Lab - APG, MASAMI NAKAGAWA, Colorado School of Mines, JUAN AGUI, NASA-Glenn Research Center, SURAJIT SEN, SUNY-Buffalo — Making shock proof layers is an outstanding challenge. Elastic spheres are known to repel softer than springs when gently squeezed but develop strong repulsion upon compression and the forces between adjacent spheres lead to *ballistic-like* energy transfer between them. Here we demonstrate for the first time that a *small alignment* of progressively shrinking spheres of a strong, light-mass material, placed horizontally in an appropriate casing, can absorb ~ 80% (~90%) of the incident force (energy) pulse. The system can be scaled down in size. Effects of varying the size, radius shrinkage and restitutive losses are shown via computed "dynamical phase diagrams."

<sup>1</sup>Supported by ARO, NSF.

Thursday, March 16, 2006 8:00AM - 11:00AM - Session U21 DFD: Liquid Crystals I Baltimore Convention Center 318

#### 8:00AM U21.00001 Aggregation in Two Dye Systems That Form Chromonic Liquid Crystals<sup>1</sup>

, PETER J. COLLINGS<sup>2</sup>, VIVA R. HOROWITZ<sup>3</sup>, MICHELLE R. TOMASIK, Department of Physics & Astronomy, Swarthmore College, Swarthmore, PA 19081 — X-ray scattering and various optical techniques are utilized to study the aggregation process and aggregate structure for two water-soluble dyes that form chromonic liquid crystal phases. The x-ray measurements indicate that the molecules stack in columns with a cross-section approximately equal to the area of a single molecule. The optical measurements point to an aggregation process that occurs at all concentrations, with the distribution of aggregate size shifting to larger and larger aggregates as the concentration is increased. A simple theory based on the law of mass action and an isodesmic aggregation process is in excellent agreement with the experimental data, yielding a value for the "bond energy" between the molecules in an aggregate.

<sup>1</sup>Partially supported by ACS-PRF Grant No. 41057-UPS

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<sup>3</sup>Present Address: Department of Physics, University of California, Santa Barbara, CA 93106

#### 8:12AM U21.00002 Orientational order of an ideal rodlike nematic: Rewriting the theory

of nematic liquid crystals? , EDWARD SAMULSKI, LOUIS MADSEN, THEO DINGEMANS, University of North Carolina - Department of Chemistry — Order in rodlike nematic liquid crystals (LCs) represents a rich field described by myriad theories and studied using various analytical methods. We have made deuterium (D) NMR observations on the labeled para-quinquephenyl LC, which closely approximates a rigid rod. To investigate this high-melting nematic (range 390 - 427 deg. C), we have fabricated a high-efficiency oven on an NMR probehead using fumed silica tiles and utilizing only ambient air cooling. Observations on p-quinquephenyl clearly and drastically deviate from the Maier-Saupe theory and all other molecular theories of nematics, thus indicating the necessity for more a complete theory (e.g., including microscopic director fluctuations) to describe nematic order. We measure the complete order tensor for this LC using combinations of quadrupole and dipolar NMR coupling constants and different D label positions. We will discuss progress on refinements to nematic order theory, relations to NMR measurements, and fits using the phenomenological Landau-deGennes theory.

8:24AM U21.00003 Interlayer interactions in ferroelectric liquid crystals<sup>1</sup>, MEHDI HAMANEH, PHILIP TAYLOR, Case Western Reserve University — We have recently drawn attention to a physical mechanism that can lead to an aligning interaction between distant layers in a ferroelectric smectic-C<sup>\*</sup> liquid crystal. This effect arises because the amplitude of thermal fluctuations in layer shape is sensitive to correlations in *c*-director orientation in layers that are not nearest neighbors. This makes the entropy of the system dependent on the relative alignment of the *c*-director in all the smectic layers. In earlier treatments of this problem, a mean-field approximation was made in order to obtain an order-of-magnitude estimate of the strength of the interlayer interaction. While this was sufficient to demonstrate the significance of the mechanism, it led to an overestimate of the overall strength of the interlayer interaction due to layer shape fluctuations. We find that the rate at which the interaction decays as a function of interlayer distance does not follow any simple power-law form, but depends on a number of material parameters.

<sup>1</sup>Research supported by PRF/ACS

8:36AM U21.00004 The B4 phase: layer curvature driven by frustrated intralayer packing, L.E. HOUGH, LCMRC, Physics Dept., CU Boulder, D. KRUERKE, Institute of Inorganic and Analytical Chemistry, TU of Berlin, C.D. JONES, LCMRC, Physics Dept., CU Boulder, H.T. JUNG, J. ZASADZINSKI, Dept. of Chemical Engineering, UCSB, G. HEPPKE, Institute of Inorganic and Analytical Chemistry, TU of Berlin, J. RABE, W. STOCKER, Institute for Physics, Humboldt U. Berlin, E. KORBLOVA, D. WALBA, LCMRC, Dept of Chemistry and Biochemistry, CU Boulder, N.A. CLARK, LCMRC, Physics Dept., CU Boulder — We combine freeze fracture transmission electron microscopy, atomic force microscopy, and x-ray diffraction to show that the B4 phase is a smectic phase with highly curved layers (mean radius ~ 4 layer spacings). The layer structure of the phase is a TGB-like phase made up of parallel arrays of multiple burgers vector screw dislocations (grain boundaries) giving 45 degree rotations across the grain boundaries. Models of the layer structure are based on periodic arrays of grain boundaries, each described by Scherk's first surface, and yield key features of the observed structures. This layered structure is dominated by saddle splay and we propose that the energy cost of defects required to make such a structure relieves the intralayer frustration produced by the packing of bent-core molecules. This work is supported by a NSF GRF and by NSF MRSEC Grant DMR0213918.

#### 8:48AM U21.00005 Polarization-Enhanced Interaction between Islands on Freely-Suspended

Smectic C\* Liquid Crystal Films<sup>1</sup>, APICHART PATTANAPORKRATANA, Department of Physics and Liquid Crystal Materials Research Center, University of Colorado, Boulder, CO 80309, U.S.A, CHEOL S. PARK TEAM, JOSEPH MACLENNAN TEAM, NOEL A. CLARK TEAM — Smectic liquid crystals can be made to form freely suspended films, two-dimensional systems locally quantized in thickness by an integral number of smectic layers, on which islands, circular regions of greater thickness than the surrounding film area, can be generated. In smectic C films, each such island is accompanied by a topological defect pair, an s = +1 topological defect inside and an s = -1 defect nearby on the background film. The distortions of the in-plane orientational order of the smectic C director field result in elastic interactions between the islands, with a short-range repulsion and a long-range dipolar attraction governing their stability and leading to their organization in chain-like structures with an equilibrium island separation. We have directly measured the repulsive and attractive forces between smectic C\* islands using multiple optical traps and have compared the results quantitatively with theory. We find that the interactions between islands are much smaller in the racemic smectic C case than in the chiral smectic C\*, an effect we attribute to long- range coulombic forces arising from polarization charges.

<sup>1</sup>This work was supported by NASA Grant NAG-NNC04GA50G and NSF MRSEC Grant No. DMR 0213918.

9:00AM U21.00006 Riverbottom texture: Patterns of compressional stress in an SSFLC cell , CHRISTOPHER D. JONES, DAVID A. COLEMAN, NOEL A. CLARK, Liquid Crystal Materials Research Center and Department of Physics, University of Colorado, Boulder, CO 80309 USA, MICHAEL D. WAND, Diplaytech, Inc., Longmont, CO 80503 USA — We have been studying the texture of remnant compressional stress in a bookshelf aligned SmA phase of the Displaytech mixture MDW8068. MDW8068 exhibits isotropic - nematic - SmA - SmC phases, and throughout the range of the SmA phase the layers show significant expansion on cooling. This layer expansion causes layer compression, which is relieved by dislocation formation and surface depinning events throughout the cell. The resulting SmA has essentially perfect alignment, but with a pattern of remnant stress that can be visualized near the SmA - SmC transition because of the divergent tilt susceptibility and resulting compression-induced tilt near the SmA - SmC transition. Low dislocation density areas are the areas of greatest layer compression, implying that the edge dislocations relieve the compressive stress. Temperature cycling shows the texture is set near the N - SmA transition, though x-ray diffraction data shows that the layer expansion occurs through the entire range of the SmA. X-ray diffraction from oriented samples has been done which shows that the texture is a result of competition between smectic ordering and surface pinning. Work supported by ED GAAN Fellowships P200A030179 and P200A000839, and NSF MRSEC Grant DMR-0213918.

9:12AM U21.00007 Random Lasing in Multidomain Cholesteric Liquid Crystals, MICHELE MOREIRA, MINGXIA GU, OLEG LAVRENTOVICH, BAHMAN TAHERI, PETER PALFFY-MUHORAY, Liquid Crystal Institute, KSU — A conventional laser consists of a pumped amplifying medium and an optical cavity to provide feedback for light amplification. In disordered materials, light can be trapped by multiple scattering processes and, if a gain medium is added, random lasing can occur. This random laser source does not require a regular cavity, but instead depends on multiple scattering in a random medium. Random lasers have attracted considerable attention recently because of their low cost and ease of construction. We present recent results of our random lasing experiments in dye-doped multidomain cholesteric liquid crystals, with submicron pitch, where the highly reflective cholesteric domains are the scattering elements. We discuss the underlying physics, compare the performance of these systems with others, consider the effects of temperature on the emission spectrum, and suggest possible applications.

9:24AM U21.00008 Wavelength Hopping in Cholesteric Liquid Crystal Lasers , MICHELE MOREIRA, CHRISTOPHER BAILEY, WENYI CAO, BAHMAN TAHERI, PETER PALFFY-MUHORAY, Liquid Crystal Institute, KSU — Due to their birefringence and periodic structure, cholesteric liquid crystals (CLCs) in the helical cholesteric phase are one-dimensional photonic band gap materials. Gain enhancement and distributed feedback effects give rise to low threshold mirrorless lasing at the band edges. Since the wavelength at the band edge is proportional to the cholesteric pitch, which is a smooth function of temperature, one would expect the lasing wavelength to vary smoothly with temperature. Observations show, however, that the lasing wavelength does not depend smoothly on temperature, but instead exhibits periodic jumps between regions of smooth monotonic behavior. We have determined the reflection band dynamics, observed multiple lasing peaks at the hopping wavelength, and see evidence of hysteresis on measuring the reflection band and lasing peaks at different heating rates. We compare our observations with theoretical models, and propose an explanation for the observed dynamics.

9:36AM U21.00009 Poisson-bracket formulation of the dynamics of polar liquid crystals<sup>1</sup>, WILLIAM KUNG, M. CRISTINA MARCHETTI, Syracuse University, KARL SAUNDERS, California Polytechnic State University — We develop the dynamical theory of polar liquid crystals with local  $C_{\infty v}$ -symmetry using the general Poisson-bracket formalism. We obtain dynamical equations for the slow macroscopic fields that govern the dynamics in both the polarized and the isotropic phases. Starting from a microscopic definition of an alignment vector proportional to the polarization, we obtain Poisson bracket relations for the director field. The hydrodynamic equations differ from those of nematic liquid crystals  $(D_{\infty h})$  in that they contain terms violating the  $n \rightarrow -n$  symmetry. We find that the  $\mathcal{Z}_2$ -odd terms induce a general splay instability of a uniform polarized state in a range of parameters.

<sup>1</sup>Work supported by NSF grants DMR- 0305407 and DMR-0219292.

#### 9:48AM U21.00010 Finite Element Elastodynamics Studies of Shape Evolution in Liquid Crys-

tal Elastomers<sup>1</sup>, ROBIN SELINGER, BADEL MBANGA, JONATHAN SELINGER, Kent State University — Liquid crystal elastomers change shape under heating/cooling, applied fields, or optical illumination, with induced strains up to 400%. We present a novel finite element elastodynamics technique to model dynamics of shape change in these materials, with explicit coupling between nematic order and elastic strain. Without added dissipation, the elastodynamics algorithm conserves the sum of kinetic and potential energy to one part in  $10^6$ , even for large strains and rotations. In initial studies, we model shape evolution during a transition from the isotropic phase to nematic and back again, and model the induced curvature of an elastomer strip under local optical illumination. This method allows modeling of complex geometries and dynamic perturbations, and can serve as a bridge between fundamental soft condensed matter theory and engineering design.

<sup>1</sup>Acknowledgment is made to the Donors of the ACS-PRF for support of this work.

#### 10:00AM U21.00011 Temperature Dependence of Acousto-Optic Effect in a Nematic Liquid

**Crystal Cell**, STEVEN SUNDBECK, ANTHONY MALANOSKI, BRIAN WESLOWSKI, DEVANAND SHENOY, United States Naval Research Laboratory, JONATHAN SELINGER, Kent State University — The acousto-optic effect occurs in a nematic liquid crystal cell when an incident ultrasonic wave causes a rotation of the director. This effect is observable as a change in the optical transmission through a cell, and has been exploited as a means of nondestructive imaging. The sensitivity and speed of this rearrangement are dependent on the viscosity of the liquid crystal material. Because of this, the effect is sensitive to the temperature. In this work we investigate quantitatively how the acousto-optic response is affected by the temperature of the liquid crystal cell. We present the results of studies of changes to the acoustic sensitivity of the cells and changes of their dynamic responses to the introduction of the ultrasonic wave.

10:12AM U21.00012 Elliptic Phases: A Study of the Nonlinear Elasticity of Twist-, CHRISTIAN SANTANGELO, RANDALL KAMIEN, University of Pennsylvania — The twist-grain boundary phase in smectic-A liquid crystals, constructed from rotating walls of parallel screw dislocations, is a prime example of a stable, ordered configuration of defects. In smectics, nonlinearities in the strains strongly affect the energetics and interactions between defects, thus complicating their analysis. By exploiting the properties of Jacobi elliptic functions, we construct a triply-periodic surface locally composed of screw dislocations, called Schnerk's surface, which has the structure of a series of ninety degree twist-grain boundaries. This is a candidate structure for the recently observed large-angle twist-grain boundary phases. Because of the analytic tractability of our construction, we compute that the grain boundaries interact exponentially at long distances through both the compression and bending energies, and that there is a preferred grain boundary spacing.

10:24AM U21.00013 Calorimetric study of aligned liquid crystal +  $aerosil^1$ , F. CRUCEANU, G. S. IANNACCHIONE, Worcester Polytechnic Institute, D. LIANG, R. L. LEHENY, Johns Hopkins University — A high-resolution ac-calorimetric study was performed on magnetically aligned colloidal dispersions of 8CB and aerosil spanning the weakly first-order *I-N* and second order *N-SmA* phase transitions. Stable aligned samples were prepared by repeated cycling between the isotropic and nematic phase in the presence of a 2 T magnetic field. Zero-field measurements were carried out on six aligned conjugate density samples ranging from 0.03 to 0.15 g cm<sup>-3</sup> (mass of aerosil per volume of liquid crystal). For comparison, two unaligned samples from the same batch (0.05 and 0.13 g cm<sup>-3</sup>) were also studied. The unaligned samples reproduce very closely previous studies on this system. The magnetically aligned samples, exhibits lower transition temperatures for the same aerosil density sample and a shift to higher aerosil density of the non-monotonic  $T_c$  evolution. The clear differences between aligned and unaligned sample indicate the "memory" of the magnetic field even after heating deep into the isotropic phase. The origin of this "memory" remains unexplained.

<sup>1</sup>Supported by NSF award DMR-0092786

10:36AM U21.00014 Disordering Effects in Smectic – Aerosil Gels\*, VISHAL PANDYA, DANIELE FINOTELLO, Kent State University — We studied quenched disorder effects on the 12CB liquid crystal upon dispersion of silica nano particles (type A-300): hydrophilic silica spheres of diameter 7nm and surface area  $S = 300 \text{ m}^2\text{g}^{-1}$ , with hydroxyl groups covering the surface. The LC-aerosil dispersions form a gel if aerosil density exceeds the percolation threshold. For low densities of aerosil dispersions and in cooling the sample, the LC director in the void volume is parallel and follows the external NMR field; a well defined and stable LC configuration forms. When a complete silica network forms and the sample orientation in the field is changed, a few silica links are broken by the field, re-aligning only a few Sm layers; the aerosil locks in the LC configuration which follows a  $P_2$  (Cos $\Theta$ ) dependence. In contrast, if the dispersion is cooled from isotropic phase outside the field, the spectra in the Sm phase is a powder pattern. The field anneals the aerosil-induced random disorder up to a certain density beyond which, disordering effects dominate; for aerosil densities greater than  $\rho_S \approx 0.055$  g/cm<sup>3</sup>, is one order of magnitude less than that in 8CB [1]. The aerosil induced disorder, quantified by the percent of LC molecules in a powder pattern, depends linearly on the density. [1] T. Jin and D. Finotello, *Phys. Rev.* E 69, 041704 (2004); *Phys. Rev Lett.* 86, 818 (2001). \*Supported by NSF-INT 03-06851, OBR B-7844 and B-7845.

#### 10:48AM U21.00015 The Effect of Aerosil Network on Smectic A-Reentrant Nematic Liquid

Crystal, MEHMET RAMAZANOGLU, SIMON LAROCHELLE, U. Toronto, ROBERT J. BIRGENEAU, U. Toronto and U.C. Berkeley — We report on a high resolution x-ray scattering study of aerosil dispersion effects on nematic-smectic A and smectic A-reentrant nematic phase transitions in 60CB (hexyloxycyanobiphenyl) and 80CB (octyloxycyanobiphenyl) liquid crystal mixtures. Dispersed aerosil particles introduce quenched randomness to the liquid crystal phases, which destroys the long range smectic order [1]. The experiment was conducted on mixtures with different 60CB:80CB concentrations and aerosil densities. The parabolic smectic A phase boundary is found to be slightly distorted in the presence of the aerosil network, with shifted transition and median ( $T_M$ ) temperatures. Above  $T_M$ , the order parameter, susceptibility and parallel correlation lengths for the thermal and random parts of the structure factor show behaviors similar to those observed in non-reentrant nematic-smectic A second order phase transitions [2]. At  $T_M$ , where the order parameter has its maximum value, the scattering peaks are only defined by the random part of the structure factor. The smectic order parameter decreases with a further decrease in temperature, while the susceptibility and thermal correlation length increasingly show nematic-like behavior. Finally, at the lowest temperature, the mixtures are found in the reentrant nematic phase. [1] P.S. Clegg et. al. PRE 67,021703 (2003) [2] S. Larochelle et. al. in preparation

#### Thursday, March 16, 2006 11:15AM - 2:15PM $_-$

Session V8 DCOMP DFD: Focus Session: Simulations Using Particles Baltimore Convention Center 314

11:15AM V8.00001 Nanoscale flows on open chemical channels , JOEL KOPLIK, City College of New York — We investigate the nano-scale flows of low-volatility liquids along "chemical channels": patterns of completely-wetting solid embedded in a planar substrate, and sandwiched between less wetting solid regions. In the case of a long, straight wetting stripe, we use molecular dynamics simulations as basic computational tool, comparing the results to a simple long-wavelength approximation and a full stability analysis based on the Stokes equations. The different approaches are qualitatively consistent, and we find that while thin liquid ridges are stable both statically and during flow, a (linear) pearling instability develops if the thickness of the ridge exceeds half of the width of the channel. In the flowing case periodic bulges propagate along the channel and subsequently merge due to nonlinear effects. However, the ridge does not break up even in the unstable case, and the qualitative behavior is unchanged when the fluid can spill over onto a partially wetting exterior solid region. For more complicated patterns involving the splitting or merger of wetting stripes, we again find that liquid flows continuously along the wetting region despite the pearling instability. In this case, intriguing switching dynamics is found for moving pearls at junctions.

 $11:51AM\ V8.00002\ Immersed\ boundaries\ and\ particles\$ , GEORGES-HENRI COTTET, Universite Joseph Fourier — This talk will present ongoing works in our group dealing with particle simulation of complex flows. We will show some non conventional particle methods to simulate incompressible elasticity and fluid-structure interactions. We will also show how particle methods in these fields, as well as for more conventional advection dominated physics, can lead to new ideas for Eulerian schemes.

12:27PM V8.00003 Particle Methods in Numerical Cosmology , HUGH COUCHMAN, McMaster University — Particle methods play a central role in numerical simulations of cosmic structure. These methods are particularly important for simulations of two-component universes that include both baryonic and "dark matter." Particles are used to model both the collisionless dark matter—using a classical inverse square law gravitational attraction—and, with Smoothed Particle Hydrodynamics (SPH), the baryonic component. Although Eulerian methods are also now widely used to model cosmological hydrodynamics, SPH exhibits many useful and important properties for cosmology: it is robust and simple to code, meshes well with the necessary particle representation of the collisionless dark matter and is able to model large density contrasts and irregular geometries easily and reliably. These methods have been used to model purely collisionless cosmic fluids with up to  $10^{10}$  particles and to model both baryonic and dark matter universes with approximately  $10^{8.5}$  particles.

12:39PM V8.00004 Fast Parallel Particle Methods: Angstroms to Gigaparsecs , MICHAEL WARREN, Los Alamos National Laboratory — Fast multipole methods have become an ubiquitous tool for the simulation of physical systems with long-range interactions. Since their introduction they have been applied to a vast range of problems. Our own parallel hashed oct-tree code (HOT) has been applied to a number of physical systems with long-range interactions, including gravitational and smoothed particle hydrodynamic interactions in astrophysical systems, fluid flows with vortex-particle methods, electromagnetic scattering and aerodynamics. Several these simulations were recognized with Gordon Bell prizes for significant achievement in parallel processing. We will discuss some recent work which used a series of 1-billion particle dark matter simulations to accurately determine the mass function of galaxy halos. These simulations required over  $4 \times 10^{18}$  floating point operations (4 exaflops). Another focus of our current research is extending the HOT framework to biological systems, with the goal of simulating systems using over ten times as many atoms as the current state-of-the-art. This requires addressing several issues with current multipole algorithms, such as spatially-correlated errors and the ability to handle disparate time scales efficiently.

12:51PM V8.00005 Efficient particle simulations based on combining the Vortex-In-Cell and the Parallel Fast Multipole methods, GREGOIRE WINCKELMANS, ROGER COCLE, GOERIC DAENINCK, Universite catholique de Louvain (UCL), FRANCOIS THIRIFAY, CENAERO and UCL — Particle methods are quality methods for simulating unsteady, convection dominated, flows, as they have negligible dissipation and dispersion. The vortex particle method is used for incompressible flows; also for buoyancy-driven flows by adding the temperature. The method can also be used for combustion, by using variable volume particles with vorticity, velocity divergence, temperature and species mass fractions. Quality particle methods also require interpolation/redistribution schemes. We here consider the Vortex-In-Cell (VIC) approach, where all operations, except convection, are done using a grid: Poisson solver, stretching, diffusion, etc. The vorticity field is also maintained divergence free by projection when required (which also requires solving a Poisson equation). In our implementation, we use the Fast Multipole method to obtain the boundary condition for solving the Poisson equation: this allows for a grid that tightly contains the particles. The method is also parallelized: the Parallel Fast Multipole (PFM) code provides the proper boundary condition on each subdomain, without iteration. Illustrative results will be presented in DNS and LES (also using multiscale models): vortex rings, wake vortices (also with ground effects), combustion.

1:03PM V8.00006 A Particle/Panel Method for Vortex Sheet Roll-Up, ROBERT KRASNY, University of Michigan — Vortex sheets are commonly used in fluid dynamics to model thin shear layers in slightly viscous flow. Some of the first Lagrangian particle simulations in fluid dynamics used the point vortex approximation to study vortex sheet roll-up. We will review the early fundamental contributions on this topic by Rosenhead, Birkhoff, and Moore, and then discuss more recent developments. In particular, a method is described for computing vortex sheet roll-up in 3D flow in which the sheet surface is represented by a set of quadrilateral panels with Lagrangian particles at the vertices. The particles are advected by a regularized Biot-Savart integral and the induced velocity is evaluated by a particle-cluster treecode. The panels are adaptively subdivided to maintain resolution as the sheet deforms. The method is applied to simulate the collision of two vortex rings. The results sheel light on the dynamics of vortex filaments in fully 3D flow.

#### 1:15PM V8.00007 Particle dynamics-based hybrid simulation of vibrated gas-fluidized beds

of cohesive fine powders , SUNG JOON MOON, YANNIS KEVREKIDIS, SANKARAN SUNDARESAN, Princeton University — We use threedimensional molecular dynamics simulations of macroscopic particles, coupled with volume-averaged gas phase hydrodynamics, to study vertically vibrated gas-fluidized beds of fine, cohesive powders. The interstitial gas flow is restricted to be effectively one-dimensional (1D) in the beds of narrow cross-sectional areas we consider. This model captures the spontaneous development of 1D traveling voidage waves, which corresponds to bubble formation in real fluidized beds. We use this model to probe the manner in which vibration and gas flow combine to influence the dynamics of cohesive particles. We find that as the gas flow rate increases, cyclic pressure pulsation produced by vibration becomes more and more significant than direct impact, and in a fully fluidized bed this pulsation is virtually the only relevant mechanism. We demonstrate that vibration assists fluidization by creating large tensile stresses during transient periods, which helps break up the cohesive assembly into agglomerates. We also study spontaneous demixing in beds of a mixture of particles of different densities, so-called the "phase separation," using an equation-free multiscale approach.

1:27PM V8.00008 Dissipative Particle Dynamics Simulations of Two-Phase Flows , ANUPAM TIWARI, JOHN ABRAHAM, School of Mechanical Engineering, Purdue University — Dissipative particle dynamics (DPD) is a coarse-grained particle method that includes thermal fluctuations. A mean-field theory based model is developed for two-phase flows. Surface tension arises in the model due to terms that account for long-range attractive forces. The model is validated through static simulations carried out to reproduce the Laplace law relationship, and dynamic simulations of liquid cylinder and drop oscillations. It is shown that in both cases analytical and computed results agree within 8%. We will also present results from simulations of capillary waves and Rayleigh-Taylor instability. In the case of capillary waves, comparisons will be shown with analytical results, and in the case of thermally induced jet breakup will also be presented.

#### 1:39PM V8.00009 Polymer chain simulations in microchannels with Dissipative Particle Dy-

**namics**, VASILEIOS SYMEONIDIS, MIT / Brown University, GEORGE KARNIADAKIS, Brown University, BRUCE CASWELL, Brown University — In this work we employ Dissipative Particle Dynamics (DPD) for simulations of dilute polymer solutions using bead-spring representations. We present comparison of two time-marching schemes: the popular velocity-Verlet and Lowe's scheme. Schmidt number effects are investigated for a series of cases, including  $\lambda$ -DNA molecules under shear (using the Marko-Siggia wormlike chain spring law) and Poiseuille flow in microchannels. Effects on the polymer depletion layer, power-law profiles and apparent viscosities are presented as a function of the number of beads per polymer chain.

#### 1:51PM V8.00010 High order viscous vortex methods with deforming elliptical Gaussians,

LOUIS ROSSI, University of Delaware, RODRIGO PLATTE, Arizona State University — Vortex methods are numerical schemes for approximating solutions to the Navier-Stokes equations using a linear combination of moving basis functions to approximate the vorticity field of a fluid. Typically, the basis function velocity is determined through a Biot-Savart integral applied at the basis function centroid. Since vortex methods are naturally adaptive, they are advantageous in flows dominated by localized regions of vorticity such as jets, wakes and boundary layers. A semi-discrete convergence formulation leads to a new viscous vortex method based on deforming elliptical Gaussian basis functions that achieves fourth order spatial convergence. One odd thing about the new method is that basis functions do not move with the physical flow velocity at the basis function centroid as is usually specified in vortex methods. Rather, high order accuracy is obtained when one adds a consistently small flow field curvature correction. We will present two distinct approaches to the evaluation of the Biot-Savart integral for elliptical Gaussian basis functions will demonstrate the efficacy of the method for both convection-diffusion problems and Navier-Stokes flows in 2D.

#### 2:03PM V8.00011 Accelerating Atomistic Molecular Dynamics Simulation in Entropic Systems

, XIN ZHOU, Los Alamos National Laboratory — The time scale of the traditional atomistic molecular dynamics simulations is too short to study wide slow dynamics of complex systems. Hyperdynamics method developed by A. F. Voter in studying of solids can not use directly in entropic systems such as fluids, biopolymers etc. By applying suitable order parameters with the symmetry of the studied systems and the characteristics of short trajectory, we build the condition of extending the hyperdynamics into fluids and algorithms. We test our results in a few modeling systems and expect the methods is used generally in simulating atomistically slow dynamics of complex fluids and biopolymers.

### Thursday, March 16, 2006 11:15AM - 2:15PM -

Session V21 DFD: Liquid Crystals II: Nano & Bio Baltimore Convention Center 318

11:15AM V21.00001 A Phenomenological Model of the Effect of Magnetic Nanoparticles and Their Surface Coating on Smectic - A Liquid Crystal Order, LUZ J. MARTINEZ-MIRANDA, University of Maryland, College Park, MD, LYNN K. KURIHARA, Naval Research Laboratory, Washington, DC, KEVIN MCCARTHEY, University of Maryland, College Park, MD, JASON HARRY, Xavier University, New Orleans, LA, ALEXIS NOEL, Morgan State University, Baltimore, MD — We studied the interaction of a smectic-A liquid crystal with magnetic nanoparticles. The behavior of smectic-A liquid crystals with magnetic particles has not been very well characterized., especially where it concerns the effect of the particles' surface coating. The effect of this termination compound on the effect the nanoparticles have on liquid crystals, smectic or nematic, has not been systematically or consistently characterized. The surface coating is needed to ensure that the particles and the smectic liquid crystals do not phase separate. The surface coating in a nanoparticle is used in biological applications to identify a particular cell. We have found out that depending on the surface coating the interaction of the nanoparticles with the liquid crystal varies. This variation is related with how the surface coating aligns the liquid crystal and how it contributes to the concentration of the nanoparticles in the liquid crystal-nanoparticle mixture. This work was partially supported by NSF grant No. NSF-DMR-0080008.

11:27AM V21.00002 Carbon nanotube liquid crystal composites<sup>1</sup>, REZA DODGE, SHIN-WOONG KANG, SATYENDRA KUMAR, Department of Physics, Kent State University, Kent, Ohio 44242, CHEOL PARK, MIA SIOCHI, National Institute of Aerospace, Hampton, VA 23666, Advanced Materials and Processing Branch, NASA Langley Research Center, Hampton, VA 23681 — The miscibility of carbon nanotubes (CNTs) in thermotropic liquid crystals is extremely low, yet they can have marked influence on the properties of their host medium. We mixed very small amounts of multi-walled CNTs in a number of cyanobiphenyl mesogens and measured the dielectric and electro-optical properties, and studied the optical textures of the composites. The homeotropic samples show a unique texture, under polarizing microscope, which indicates that the nanotubes behave as line singularities with the strength of +1. The distorted alignment around these singularities covers a limited range, which is comparable with the sample thickness. The results of experiments on composites with various concentrations of CNT will be presented.

<sup>1</sup>Supported by NASA Langley Research Center through grant # NNL04AA14A.

11:39AM V21.00003 Organization of Magnetic Nanowires via Elastic Forces in a Periodic Multi-Domain Nematic Liquid Crystal<sup>1</sup>, CLAYTON LAPOINTE, DANIEL REICH, ROBERT LEHENY, Johns Hopkins University — An anisotropic particle suspended in a thermotropic nematic liquid crystal imposes an elastic energy cost on the nematic that depends on the orientation of the particle relative to the nematic director. In a nematic with a spatially varying director field, such a particle can hence experience translational forces that depend on its orientation. We report experiments in which we exploit these forces to organize ferromagnetic Ni nanowires suspended in the nematic 4-pentyl-4-cyanobiphenyl (5CB). Using lithographic techniques to pattern the nematic anchoring conditions on substrates, we generate periodic multi-domain nematic environments for the wires. With their orientation controlled by a small external magnetic field, the wires sediment to preferred domains to minimize elastic energy.

<sup>1</sup>Johns Hopkins University

11:51AM V21.00004 Liquid Crystal Alignment Induced by a Magnetic Field and the Associated Surface Memory Effect<sup>1</sup>, RUI GUO, QINGBING WANG, SATYENDRA KUMAR, Department of Physics, Kent State University, Kent, Ohio 44242, YURI REZNIKOV, Institute of Physics of National Academy of Science, Prospect Nauki 46, Kyiv 252022, Ukraine — Nematic liquid crystals, 4, 4'-n-pentylcyanobiphenyl (*5CB*) and a commercial mixture, *E*7, have been found to align in thin cells prepared by cooling from the isotropic phase in the presence of a strong magnetic field parallel to the ITO coated glass substrates. The field induced alignment is very stable and possesses surface memory effect [1]. Surprisingly, the azimuthal anchoring energy is as high as  $10^{-3}$  erg/cm<sup>2</sup> and comparable to that obtained for rubbed polymer alignment layers. The surface memory effect is thermally stable and cannot be erased even after holding the cell more than 40K above the clearing point for up to two hours. We believe that the magnetic field directed rearrangement of the LC molecules adsorbed [2] at the substrate is responsible for the observed behavior. — [1]. N. A. Clark, Phys. Rev. Lett. **55**, 292 (1985). [2]. Y. shi, B. Cull, and S. Kumar, Phys. Rev. Lett. **71**, 2773 (1993).

<sup>1</sup>Supported by the National Science Foundation grant DMI-04-23619.

#### 12:03PM V21.00005 The Study of the Fluorescent Spectrum of Cd-Se Quantum Dots in Liquid

 $Crystal Cell^1$ , YU-SUNG LIN, Department of Physics, National Sun Yat-sen University, Kaohsiung, 804, Taiwan, WEN-CHI HUNG, WOOD-HI CHENG, Institute of Electro-Optical Engineering, National Sun Yat- sen University, Kaohsiung, 804, Taiwan, I-MIN JIANG, Department of Physics, National Sun Yat-sen University, Kaohsiung, 804, Taiwan, MING-SHAN TSAI, Department of Applied Physics, National Chiayi University, Chiayi, 600, Taiwan — We report the analysis of the fluorescent spectrum of Cd-Se quantum dots in liquid crystal matrices. The cell is filled with the commercial liquid crystal (E7) in homogeneous alignment. We can vary the director field orientation of liquid crystals by applying electrical fields. With a light source of a xenon lamp to excite the Cd-Se quantum dots, the effect on the fluorescent spectrum due to liquid crystal environment is then explored. The shift of fluorescent spectrum affected by the concentration of Cd-Se quantum dots is also discussed in the report. Then the Cd-Se quantum dots are excited by use of a monochromatic Nd-YAG laser, which is a polarized light source. We explore the effects of polarization on fluorescent spectrum of Cd-Se quantum dots also.

<sup>1</sup>National Science Council of Taiwan, R.O.C. NSC94-2112-M-110-013

12:15PM V21.00006 Transmissive Fabry-Perot Spectrum of Liquid Crystal Device for measuring the Surface Plasmon Effect of Silver nano-Particle<sup>1</sup>, WEN-CHI HUNG, Inst. of Electro-Optical Engr., Natl. Sun Yat-sen Univ., Taiwan, YU-SUNG LIN, Dept. of Physics, Natl. Sun Yat-sen Univ., Taiwan, MING-SHAN TSAI, Dept. of Applied Physics, Natl. Chiayi Univ., Taiwan, I-MIN JIANG, Dept. of Physics, Natl. Sun Yat-sen Univ., Taiwan, WOOD-HI CHENG, Inst. of Electro-Optical Engr., Natl. Sun Yat-sen Univ., Taiwan, — A Fabry-Perot scheme for measuring the surface plasmon effect of Ag nano-particles has been presented. As an optical spectrum ananlyzer, the resolution of the Fabry-Perot etalon.is determined by the morphology of reflectors and resonated cavity of the etalon. Ag nano-particles of size 50 nm are deposited on the surfaces of two reflectors. The cavity is filled with liquid crystals which are homogeneous alignment. Because the surface plasmon effect (SPE) of metal nano particles is sensitive to the polarization of incident light (P-wave or S-wave), we apply various polarization lights to explore the spectra of Fabry-Perot etalon filled with liquid crystal to study the SPE of metal nano-particles. In the transmissive spectra, we find the wavelength shift at the peak (603 nm) is about 8 nm when the probed light is changed from P-wave to S-wave. Comparing the measurements of the etalon without filled with the liquid crystal; we discuss the correlation of the wavelength shift and SPE of Ag nano-particles in the liquid crystal etalon device.

<sup>1</sup>National Science Council of Taiwan, R.O.C. NSC94-2112-M-110-013

#### 12:27PM V21.00007 Investigating mixtures of rotor molecules and liquid crystals by dielectric

**spectroscopy and optical microscopy**, DEBRA KRAUSE, CHARLES T. ROGERS, Dept. of Physics, University of Colorado, Boulder, JOSE E. NUNEZ, MIGUEL GARCIA-GARIBAY, Dept. of Chemistry and Biochemistry, University of California, Los Angeles — Rotor molecules are fundamental in nanotechnology. These molecules are synthesized with one part of the molecule designed to freely rotate while other parts are attached to a surface or within a crystalline state have shown that steric interactions between neighboring molecules can result in large energy barriers (up to 21 kcal/mol) that inhibit motion of the rotor. In an effort to free the rotor but maintain degrees of order in position and orientation, we mix these molecules with liquid crystals, particularly those based on benzylidene-(4-phenylazo-phenyl)-amine. The rotor molecules can dissolve in these liquid crystals into solutions of up to 20 percent by mass. To characterize the environment of the rotor, we study the mixtures using dielectric spectroscopy and optical microscopy.

#### 12:39PM V21.00008 Flexible plastic cells fabricated using phase separation of liquid crystal

from its mixture in a prepolymer<sup>1</sup>, QINGBING WANG, RUI GUO, SATYENDRA KUMAR, Department of Physics, Kent State University, OH 44240 — During phase separation of liquid crystal (LC) from its mixture in a prepolymer, in a cell, the prepolymer accumulates near the spacers. After the phase separation is complete, UV irradiation is used to crosslink the polymer thereby fixing the position of the spacers and bonding them to the substrates. We employ this method to create polymer-embedded spacers to improve cell gap uniformity for LC displays using plastic substrates. Spacers remain adhered to their initial positions thus preventing them from movement or aggregation during temporary cell deformation. Scanning electron microscopy was employed to evaluate the internal polymer morphologies formed under different polymerization conditions. Electro-optical performances and the flexibility of plastic LC cells were determined and the details will be presented.

<sup>1</sup>Supported by a grant from Samsung Electronics Corporation

#### 12:51PM V21.00009 Adding Mono- and Multivalent Ions to Lyotropic Chromonic Liquid Crys-

**tals**, LUANA TORTORA, HEUNG-SHIK PARK, KELLY ANTION, CHRIS WOOLWERTON, DANIELE FINOTELLO, OLEG LAVRENTOVICH, Kent State University — Lyotropic Chromonic Liquid Crystals (LCLCs) are a distinct class of liquid crystals formed in aqueous solutions by molecules with rigid polyaromatic cores and ionic groups at the periphery [1-4]. The phase diagrams of these materials should depend on entropic factors (as in the Onsager model) and electrostatic interactions. Using optical polarizing microscopy, we studied the effects of mono- and multivalent ions on the phase diagrams of Blue 27 [3] and Sunset Yellow [2]. The monovalent ions change the temperatures of phase transitions, as described in [4], while the effect of multivalent ions is more dramatic and, in addition to the changed temperatures of phase transitions by tens of degrees, it often involves condensation of LCLC aggregates into domains with birefringence much higher than that in a normal nematic phase. Work supported by OBR B-7844. [1]J. Lydon, *Current Opin. Colloid & Interface Sci.* 3, 458 (1998);8, 480-489 (2004); [2]V. R. Horowitz, L. A. Janowitz, A. L. Modic, P. J. Heiney, and P. J. Collings, 2005, *Phys. Rev. E* 72, 041710; [3]Yu. A. Nastishin, H. Liu, T. Schneider, T., V. Nazarenko, R. Vasyuta, S. V. Shiyanovskii, and O. D. Lavrentovich, 2005, *Phys. Rev. E* 72, 041711; [4]A.F. Kostko, B. H. Cipriano, O. A. Pinchuk, L. Ziserman, M. A. Anisimov, D. Danino, and S. R. Raghavan. J. Phys. Chem. B 109, 19126-19133 (2005)

#### 1:03PM V21.00010 Building Shape Surfactants: Creating rod-coil complexes using genetically

engineered viruses, PHIL HUANG, SETH FRADEN, Brandeis University — Complex self-assembled structures (micelles, lamellar phases) are often found in dispersions of amphiphilic molecules like surfactants. We genetically engineered M13 bacteriophage, a long filamentous particle that forms liquid crystalline phases, and coupled a 15 base pair oligonucleotide to one end of the virus. A plasmid DNA fragment was then ligated to the oligonucleotide to form a rod-coil particle. Based on the above complex conjugate, we are attempting to create supramolecular liquid crystalline structures.

1:15PM V21.00011 Stretching the limits of membrane charge density using Dendrimer Lipids - New Highly Transfecting Hexagonal Phases for Gene Delivery, KAI EWERT, ALEXANDRA ZIDOVSKA, HEATHER M. EVANS, CYRUS R. SAFINYA, Materials, Physics, and Molecular, Cellular and Developmental Biology Departments, UCSB, Santa Barbara, CA 93106 — Newly designed multivalent lipids ranging in head group charge from 4+ to 16+ have been synthesized and investigated as DNA delivery vectors. These dendritic lipids (DLs) allow a controlled study of the relationship between membrane charge density ( $\sigma$ ) and transfection efficiency (TE). An earlier report from our group described that TE of different cationic lipids of charge 1+ to 5+ follows a common, bell shaped curve as a function of membrane charge density [1]. To further probe this universal behavior, the dendritic lipids with higher valence were designed in order to reach higher values of  $\sigma$ . Structural studies using x-ray diffraction reveal new phases, where cylindrical micelles of DLs form a hexagonal lattice which holds together a continuous DNA network, described as H<sup>C</sup><sub>I</sub> [2]. The new hexagonal phase is highly transfecting in the regime where the TE of lamellar complexes follows a decrease in the bell curve. Small angle x-ray scattering studies have revealed a rich phase diagram of micelles made from DL/DOPC mixtures. Funding provided by NIH GM-59288 and NSF DMR-0503347. [1] A. Ahmad et al., J. Gene Med., 2005, V7:739-748. [2] K. Ewert et al., J. Am. Chem. Soc., (submitted).

## 1:27PM V21.00012 Hollow Rectangular Columnar Structure in Dendritic Supramolecular Assemblies<sup>1</sup>, MIHAI PETERCA, PAUL HEINEY, Dept. of Physics, Univ. of Pennsylvania, MARC ILIES, ANDRES DULCEY, SAMI NUMMELIN, VIRGIL PERCEC, Dept. of Chemistry, Univ. of Pennsylvania — Hollow columnar phases have recently attracted interest for their potential applications as channel mimics in membrane transport, as photonic band gap materials, and for selective encapsulation. The first dendritic structures that self-assemble into hollow rectangular phases have been synthesized and a method for their structural analysis by x- ray diffraction experiments has been developed. The structural analysis method developed allows the calculation of the pore separation, shape and size, creating new opportunities for separation processes of symmetric or asymmetric compounds.

<sup>1</sup>Supported by the MRSEC program of the National Science Foundation under award # DMR05-20020.

# 1:39PM V21.00013 X-Ray Determination of the Structure and Phases of Liquid Crystals of Nanoscale Duplex DNA, MICHI NAKATA, U. of Colorado, GIULIANO ZANCHETTA, U. of Milano (IT), CHRISTOPHER JONES, U. of Colorado, BRANDON CHAPMAN, Brookhaven National Lab., RONALD PINDAK, Brookhaven National Lab., TOMMASO BELLINI, U. of Milano, NOEL CLARK, U. of Colorado — Polymeric DNA chains are known to exhibit chiral nematic and hexagonal columnar LC phases. Recently we found that even very short duplex B-DNA oligomers 6-basepairs (bp) to 16-bp in length also form nematic and columnar phases depending on the concentration of DNA. To investigate the structure of those phases, we used micro-beam x-ray diffraction (10 micron spot size), enabling the study of single LC domains. In the columnar phases of 8bp, 12bp and 16bp all shows reflection spots corresponding to 20/AA which almost the same length scale of the width of DNA double helix. By selecting a proper orientation of the domains the diffraction pattern shows a hexagonal packing of columns of spacing which does not depend on the length of the basepair. On the other hand, there is no clear diffraction in the chiral nematic phase, which indicates that there is no significant highly ordered molecular aggregation. Those data indicate that short oligomers stack end- to end to form flexible rod-shaped DNA aggregates can then form LC phases. Work supported by NSF MRSEC Grant DMR 0213918 and NSF Grant 0072989.

1:51PM V21.00014 Probing the mechanical unzipping of DNA, NIKOS K. VOULGARAKIS, ALAN R. BISHOP, KIM O. RASMUSSEN, Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — Recent advances in single-molecule force spectroscopy have made a systematic study of local melting in DNA possible. This provide new insight into important biological processes as replication and transcription. In this work, we present an extensive study of the micromechanical unzipping of DNA in the framework of the Peyrard-Bishop-Dauxois (PBD) model. The force required to separate the doubled strand is derived through analysis of the force-extension curve, while an estimation of the nucleation bubble size of the unzipping process is obtained by the distribution of the rapture force. Our findings are in very good agreement with existing experimental results; for example the force-temperature phase diagram obtained by the PBD model agrees excellently with recent constant-force experimental measurements of the lambda-phage DNA. Fundamental differences between the in vivo and vitro DNA unzipping, as predicted by the PBD model, are also discussed.

2:03PM V21.00015 Asymmetrical binding of cationic peptides onto an oppositely-charged lipid-bilayer membrane: area expansion and membrane rupture<sup>1</sup>, SATTAR TAHERI-ARAGHI, BAE-YEUN HA, Department of Physics, University of Waterloo, Ontario N2L 3G1, Canada — We study asymmetrical binding of cationic peptides onto a negatively charged lipid-bilayer membrane. The peptide not only interacts electrostatically with anionic lipids, rearranging their spatial distributions, but it can also insert hydrophobically into the membrane, expanding the area of its binding layer (i.e., the outer layer). We examine how peptide charges and peptide insertion (thus area expansion) are intertwined. Our results illustrate why high valences are required for selective toxicity of antimicrobial peptides, (i.e., they selectively rupture bacterial membranes while leaving host cells intact).

<sup>1</sup>This work was supported by the Natural Sciences and Engineering Research Council of Canada

## Thursday, March 16, 2006 2:30PM - 5:30PM -

Session W8 GSNP DFD: Focus Session: Nonlinear Electrokinetics Baltimore Convention Center 314

2:30PM W8.00001 Electro-Convective and Non-Equilibrium Electro-Osmotic Instability of Electric Conduction from an Electrolyte Solution into a Charge Selective Solid, ISAAK RUBINSTEIN, Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev — Electro-convection is reviewed as a mechanism of mixing in the diffusion layer of a strong electrolyte adjacent to a charge-selective solid, such as an ion exchange (electrodialysis) membrane or an electrode. Two types of electro-convection in strong electrolytes may be distinguished: bulk electro-convection , due to the action of the electric field upon the residual space charge of a quasi-electro-neutral bulk solution, and convection induced by electro-osmotic slip, due to electric forces acting in the thin electric double layer of either quasi-equilibrium or non-equilibrium type near the solid/liquid interface. According to recent studies, the latter appears to be the likely source of mixing in the diffusion layer, leading to 'over-limiting' conductance in electroilayis. Electro-convection near a uniform charge selective solid/liquid interface sets on as a result of hydrodynamic instability of one-dimensional steady state electric formulations. The short- and long-wave aspects of these instabilities are discussed along with the wave-number selection principles and possible sources of low frequency excess electric noise experimentally observed in these systems.

**3:06PM W8.00002 Nonlinear Surface Transport in the Thin Double-Layer Limit**, KEVIN CHU, Princeton University, MARTIN BAZANT, Massachusetts Institute of Technology — At high applied electric fields, ionic transport within the double layer plays a significant role in the overall response of electrokinetic systems. It is well-known that surface transport processes, including surface electromigration, surface diffusion and surface advection, may impact the strength of electrokinetic phenomena by affecting both the zeta-potential and the magnitude of the tangential electric field. Therefore, it is important to include these effects when formulating the effective boundary conditions for the equations that govern electrokinetic flow outside of the double layer. In this talk, we discuss the application of a general formulation of "surface conservation laws" for diffuse boundary layers to derive effective boundary conditions that capture the physics of electrokinetic surface transport. Previous analyses (*e.g.* Deryagin & Dukhin 1969) are only valid for weak applied fields and are based on a linearization of the concentration and potential about a reference solution, but our results are fully nonlinear and hold at large applied fields as long as the double layer is sufficiently thin. We compare our nonlinear surface transport theory with existing linear analogues and apply it to the canonical problem of induced-charge electro-osmosis around a metal sphere or cylinder in a strong DC field.

**3:18PM W8.00003 Experiments on Nonlinear Electrokinetic Pumps in Microfluidics**<sup>1</sup>, JOHN PAUL URBANSKI, TODD THORSEN, Department of Mechanical Engineering, MIT, JEREMY A. LEVITAN, MARTIN Z. BAZANT, Department of Mathematics, MIT — Nonlinear electrokinetic pumps are attractive in the development of portable and flexible microfluidic analysis systems, since they operate without moving parts using low (battery powered) alternating potentials. Since the discovery of AC electro-osmosis (ACEO) in the late 1990s, there has been much work in designing and building two-dimensional, periodic micro-electrode geometries, which exploit broken symmetry to rectify AC forcing and produce steaming flow over a surface. Building on this work, we exploit more general principles of induced-charge electro-osmosis (ICEO) in three-dimensional electrode geometries to enhance pumping in microfluidic devices. Our fabrication efforts are guided by theoretical analysis and simulations using the standard low-voltage theory, which, in some cases, predict flow rates faster than existing planar ACEO pumps by an order of magnitude (for the same voltage and feature size). We test various microfabricated pump geometries in a microfluidic loop following the methodology of Studer et al (2004). We are also measuring the strong effect of solution chemistry (e.g. ion valence and concentration) on ICEO flow to guide further developments in the theory of nonlinear electrokinetics.

<sup>1</sup>Supported by the US Army through the Institute for Soldier Nanotechnologies.

#### 3:30PM W8.00004 Microfluidic pumps based on Induced Charge Electroosmosis and flow Field

Effect Transistor phenomena<sup>1</sup>, GAURAV SONI, TODD SQUIRES, CARL MEINHART, University of California Santa Barbara — We are developing AC electrokinetic micropumps to drive electrically conductive biological fluids in microchannels. These pumps work on the principles of Induced Charge Electroosmosis (ICEO) and flow Field Effect Transistor (flowFET) phenomena. AC (as well as DC) electric fields can induce electrical double layer on a polarizable surface and in turn, cause fluid motion by moving this layer. However, when the polarizable surface is electrically floating, symmetric vortices are observed on the surface. Symmetry of this flow leads to zero net pumping. In order to achieve pumping, we apply a second AC signal to the polarizable surface. When the magnitude of this second AC signal is different from the floating potential of the surface, unidirectional flow is observed i.e., pumping is achieved by modulating the induced zeta potential of the surface. Pumping caused by modulation of zeta potential is also known as flowFET phenomenon and has been shown to work with DC electric fields by other community members. We show a detailed study of flowFET with AC electric fields.

<sup>1</sup>Supported by an Army grant: 8-487859-25500.

3:42PM W8.00005 Nonlinear studies of AC electrokinetic micropumps , HENRIK BRUUS, LAURITS H. OLE-SEN, Technical University of Denmark, ARMAND AJDARI, Ecole Superieure de Physique et de Chimie Industrielles — Recent experiments have demonstrated that AC electrokinetic micropumps permit integrable, local, and fast pumping (velocities  $\sim$  mm/s) with low driving voltage of a few volts only. However, they also displayed many quantitative and qualitative discrepancies with existing theories. We therefore extend the latter theories to account for three experimentally relevant effects: (*i*) vertical confinement of the pumping channel, (*ii*) Faradaic currents from electrochemical reactions at the electrodes, and (*iii*) nonlinear surface capacitance of the Debye layer. We report here that these effects indeed affect the pump performance in a way that we can rationalize by physical arguments. **3:54PM W8.00006 Electric field driven motion of flexible polyelectrolytes**<sup>1</sup>, TAK SHING LO, Levich Institute, City College of CUNY, BORIS KHUSID, Dept. of Mechanical Engineering, NJIT, ANDREAS ACRIVOS, JOEL KOPLIK, Levich Institute, City College of CUNY — Our work aims to study dielectrophoresis of biomolecules in micro/nano-fluidics using molecular dynamics (MD) simulations. Our model combines electrohydrodynamics with molecular theories for the macromolecule polarization caused by the distortion of the counterion cloud. Unlike most available MD studies of polyelectrolytes, solvent atoms are explicitly represented in our model, so that hydrodynamic interactions are included naturally with no ad hoc assumption. The polyelectrolyte is modeled as a negatively charged bead-spring chain. The charges interact through the Coulomb potential and other molecular interactions are included via Lennard-Jones potentials. We study the transport properties of flexible polyelectrolytes suspended in a solvent, with or without added salt, under the action of DC or AC electric fields. MD data provide the information needed to compute the dipole moments of the molecule and the surrounding double layer, which are required for understanding the dielectrophoretic behavior of these molecules in nanoscopic channels.

<sup>1</sup>This work was supported by NSF (CTS-0307099) and NSF/Sandia (NIRT/NER-0330703).

4:06PM W8.00007 Anomalous ionic transport at nanometer-scale electrodes, DIEGO KRAPF, Deft University of Technology, BERNADETTE QUINN, MENG-YUE WU, HENNY ZANDBERGEN, CEES DEKKER, SERGE LEMAY — We probe the transport of charged species in high ionic strength solutions on the scale of a few nanometers by monitoring electrochemical reactions at correspondingly sized electrodes. The electrical current through the nanoelectrode provides a direct measure of the flux of ions across the diffuse double layer. Because both the concentration gradient and the electric field are localized in the immediate vicinity of the nanoelectrode, this provides very local information. Furthermore, when the electrode dimensions are in the order of a few nanometers, very steep concentration gradients are achieved. To carry out these experiments, we have developed a method for fabricating nanoelectrodes with a well-defined size and geometry. A pore is first drilled in an insulating membrane with a focused electron beam and it is then filled with a noble metal yielding conically shaped, convex electrodes with radii as small as 2 nm. We observe pronounced non-linearities of ion flux versus concentration when transport is localized within a region smaller than 10 nm in size. We numerically calculate the predicted ion flux using the Stern-Poisson-Nernst-Planck formalism. We show that our observations cannot be explained using this widely applied mean-field description of ionic transport.

4:18PM W8.00008 Nonlinear Electroosmosis and Biomolecule Electrokinetic Trapping Induced by Ion Selective Nanofluidic Channels, YING-CHIH WANG, Dept. of Mech. Eng., MIT, JONGYOON HAN, Bio. Eng. Division, Dept. of EECS, MIT — This paper describes a nanofluidic device that can concentrate dilute biomolecule by electrokinetic trapping mechanism. This device has nanofluidic channels with a depth down to 40 nm, therefore, having significant Debye layer overlap. Depending on the strength of the applied potential across the nanochannel, one can observe phenomena such as concentration polarization; charge depletion and nonlinear electrokinetic flow in the adjacent microfluidic channel using fluorescent microscopy. By manipulating the electric field, the device can generate an extended space charge region, maintained for several hours, within a microchannel as a mean to collect and trap biomolecules. Our studies demonstrate such device can achieve up to 10 million fold sample preconcentration within 30 minutes. Besides, if applied a higher potential, a much faster chaotic flow can be seen in the microchannel adjacent to nanochannels. This kind of nonlinear electrokinetic flow is often called the electrosmosis of the second kind or induced-charge electroosmosis in electrode and ion exchange membrane studies. The presented device can be used as either a preconcentrator or an injector to other separation and detection systems preferred its performance and integrabilty. Also, it is an ideal experimental platform for studying such nonlinear electrokinetic effects, by directly tracking molecules *in situ.* 

4:30PM W8.00009 Modeling of Selectively Permeale Vesicle Membrane in Electrolytes: An Energetic Variational Formulation, CHUN LIU, ROLF RYHAM, Dept of Math, PSU — We introduce a self consistent coupled system to model the deformation of selectively permeable vesicle membranes in electrolytes via an energetic variational formulation. The equations governing a diffuse charge system and the evolution of the vesicle membrane are coupled with the momentum equations of the electrolyte through the Lorentz force along with the induced elastic forces due to the membrane bending energy. The force coupling and charge flux selectivity are consequences of the energetic balance and competition of kinetic, electric and membrane elastic bending energy. We will also present some numerical simulation results of the system.

#### 4:42PM W8.00010 Reversible Transitions on Electrically-Tunable Nanostructured Superhy-

**drophobic Surfaces**, TOM KRUPENKIN, J. ASHLEY TAYLOR, PAUL KOLODNER, MARC HODES, JOANNA AIZENBERG, Bell Labs, Lucent Technologies — Recently demonstrated electrically tunable nanostructured superhydrophobic surfaces provide a promising new way of manipulating liquids at both micro and macro scales. Dynamic control over the interaction of liquids with the solid substrate is of great interest to many research areas ranging from biology and chemistry to physics and nanotechnology. In this work the reversibility of the electrically induced superhydrophobic – hydrophilic transition on nanostructured surfaces is addressed. Recently demonstrated approach based on momentarily induction of film boiling in a very thin layer of liquid adjacent to the solid-liquid interface is discussed. The dependence of the hydrophilic – superhydrophobic transition on the topography of the nanostructured layer, as well as on the energy and duration of the electrical pulse is investigated. Several emerging applications of these surfaces, including lab-on-a-chip, chemical microreactor, and on-chip power sources are discussed.

#### 4:54PM W8.00011 Nonlinear alternating current susceptibilities of rotating microparticles in

electrorheological fluids<sup>1</sup>, KIN WAH YU, Chinese University of Hong Kong, J.P. HUANG, W.J. TIAN, Fudan University — A perturbation approach [1] has been employed to investigate the nonlinear alternating current (AC) responses of the rotating microparticles in electrorheological (ER) fluids under AC or direct current electric fields. The shear flow of ER fluids exerts a torque on the particles and leads to the rotational motion of the particles about their centers [2]. We show that the dynamic effects can play a significant role in the AC responses. Our results can be conveniently interpreted in the dielectric dispersion spectral representation [3], thus offering a convenient method to determine the relaxation time and the rotation velocity of the ER particles by measuring the nonlinear AC responses.

[1] G. Q. Gu and K. W. Yu, Phys. Rev. B 46, 4502 (1992); K. W. Yu, P. M. Hui, and D. Stroud, Phys. Rev. B 47, 14150 (1993).

[2] Jones T. K. Wan, K. W. Yu, and G. Q. Gu, Phys. Rev. E 62, 6846 (2000).

[3] Jun Lei, Jones T. K. Wan, K. W. Yu, and Hong Sun, Phys. Rev. E 64, 012903 (2001).

<sup>1</sup>Work supported by RGC Earmarked Grant

5:06PM W8.00012 Electrophoresis in bounded doamins, EHUD YARIV, Technion — Electrophoretic motion is usually described by a linear model, based upon the smallness of the applied field relative to the equilibrium field in the screening Debye layer surrounding the particle. This model, in turn, leads to the Smoluchowski's slip condition and eventually results in mobility relations. The mobility concept is valid provided the external electric force is neglected — a procedure superficially supported by the net electric neutrality of the combined particle-layer system. In this talk, however, I will show that this force does not vanish in general. Accordingly, a consistent scheme is formulated for analyzing the nonlinear motion of a particle in an applied field. This motion is illustrated in two contexts: rotation of non-spherical particles, and drift of a spherical particle away from a planar wall. I will also describe an analogy to incompressible and inviscid fluid motion. This analogy enables for experimental verification of three-dimensional potential flow solutions.

5:18PM W8.00013 How accurate is the Poisson-Boltzmann theory for monovalent ions near highly charged interfaces?<sup>1</sup>, WEI BU, ALEX TRAVESSET, DAVID VAKNIN, Ames Laboratory, Iowa State University — Monovalent ion distributions next to highly charged interfaces were determined by synchrotron surface X-ray sensitive techniques. A lipid phosphate (dihexadecyl hydrogenphosphate) was spread as a monolayer at the air-water interface, containing CsI at various concentrations. Using anomalous reflectivity off and at the  $L_3$  Cs<sup>+</sup> resonance, we provide, for the first time, spatial counterion distributions (Cs<sup>+</sup>) next to the negatively charged interface over a wide range of ionic concentrations. We argue that at low salt concentrations and for pure water the enhanced concentration of hydroniums H<sub>3</sub>O<sup>+</sup> at the interface leads to proton-transfer back to the phosphate group by a high contact-potential, whereas high salt concentrations lower the contact-potential resulting in proton- release and increased surface charge-density. The experimental ionic distributions are in excellent agreement with a renormalized-surface-charge Poisson-Boltzmann theory without fitting parameters or additional assumptions.

<sup>1</sup>The MUCAT sector at the APS and the use of the APS are supported by the U.S. DOE, Basic Energy Sciences through Ames Laboratory under Contracts No. W-7405-Eng-82, and No. W-31-109-Eng-38, respectively.

## Thursday, March 16, 2006 2:30PM - 5:30PM -

Session W21 DFD: Liquid Crystals III Baltimore Convention Center 318

2:30PM W21.00001 Dielectric Dispersion Effects in Liquid Crystals.<sup>1</sup> , OLEG LAVRENTOVICH, Liquid Crystal Institute, Kent State University, YE YIN, MINGXIA GU, SERGIJ SHIYANOVSKII — As the switching speed in practical LC devices is pushed from the currently common 10 ms to sub-millisecond levels, it is important to take into account the effects associated with the finite rate with which the electric displacement changes in the external electric field. We discuss two important general consequences of the dielectric relaxation phenomenon: (1) Non-local time relationship between the electric displacement and the electric field [1]. In a quickly changing electric field, orientation of the liquid crystal depends not only on the instantaneous value of the electric field, but also on the previous values of the field and previous orientations of the material. (2) Dielectric heating. [1] Y. Yin, S.V. Shiyanovskii, A.B. Golovin, and O. D. Lavrentovich, Phys. Rev. Lett. 95, 087801 (2005) .

<sup>1</sup>Work partially supported by NSF DMR0315523

#### 2:42PM W21.00002 Using micro-focus synchrotron X-ray diffraction to probe textured liquid

crystal samples<sup>1</sup>, RONALD PINDAK, BRANDON CHAPMAN, Brookhaven National Lab, RUITING WANG, ISHTIAQUE SYED, GIOVANNI CAR-BONE, CHARLES ROSENBLATT, Case Western Reserve Univ., MICHI NAKATA, CHRISTOPHER JONES, NOEL CLARK, Univ. of Colorado, SHIN-WOONG KANG, Kent State Univ., SATYENDRA KUMAR, National Science Foundation, JULIE CROSS, Argonne National Lab — 16 KeV X-rays from a bend magnet source at Sector 20 of the Advanced Photon Source were micro-focused by Kirkpatrick-Baez mirrors to a 14µm × 14µm cross-section and used in conjunction with an in-situ polarizing optical microscope to measure the diffraction from select areas in textured liquid crystal samples between thin glass plates. The technique will be described and its utility illustrated by three examples: (1) measuring the orientational deformation of smectic-A liquid crystal layers under the bend strain imposed by an AFM-scribed polymer alignment film, (2) mapping the concentration dependence of the liquid crystal phases exhibited by suspensions of short DNA oligomers of 6 to 16 base-pairs, and (3) selecting local monodomain regions from a globally unaligned conducting porphyrin-derivative sample for structural determination of its liquid crystal phases.

<sup>1</sup>supported in part by the U.S. Department of Energy under grant No. 04SCPE389

2:54PM W21.00003 Impurity Induced Cross-over from Continuous to First-order Nematic-to-Smectic A Phase Transitions in a Liquid Crystal., Jan Thoen, Katleen denolf, Bert van Roie, Christ Glorieux, Lab. Akoestiek en Thermische Fysica, Dept. Natuurkunde en Sterrenkunde, Katholieke Universiteit Leuven, Celestijnenlaan 200 D, B-3001 Leuven, Belgium - We used adiabatic scanning calorimetry (ASC) to study the impact of adding small amounts of cyclohexane on the N-SmA transition of the liquid crystal octylcyanobiphenyl (8CB). The transition remains continuous upto a mole fraction of cyclohexane near 0.05, where at a tricritical point the transition becomes first- order with latent heats increasing with mole fraction of cyclohexane. Along the continuous part of the N-SmA transition line the effective specific heat capacity critical exponent increases from 0.31 for 8CB to 0.50 at the tricritical point. Ongoing experiments with other non-mesogenic impurities will also be reported.

3:06PM W21.00004 Phase morphology of a disk-sphere dyad molecule. , LI CUI, JEFFREY COLLET, LEI ZHU, Polymer Program, Institute of Materials Science and Department of Chemical Engineering, The University of Connecticut, Storrs, CT 06269-3136 — A disk-sphere dyad molecule was synthesized by attaching a discotic triphenylene molecule to a spherical polyhedral oligomeric silsesquioxane (POSS) molecule via esterification reaction. The self-assembly behavior of the dyad molecule was studied by differential scanning calorimetry, polarized light microscopy, X-ray diffraction (XRD), and transmission electron microscope. Two-dimensional (2D) XRD results showed the dyad molecules self-assembled into a lamellar structure, which composed of a crystalline POSS layer and a discotic-nematic triphenylene double-layer. The POSS layer consisted four layers of ABCA-stacked spherical molecules. The liquid crystalline triphenylene molecules were parallel and staggered in the double-layer. Computer simulation of the XRD intensity confirmed the proposed structural model. Compared with that of the POSS crystal in bulk (melting point at ca 220 °C), the melting temperature of POSS crystal was dramatically decreased to 67 °C, possibly due to effects of the asymmetry molecular shape and plasticization of the discotic triphenylene moieties between POSS lavers.

#### 3:18PM W21.00005 Excitation-Enhanced Optical Reorientation in Pure Liquid Crystalline

Materials , THAI V. TRUONG, YUEN-RON SHEN, Department of Physics, University of California, Berkeley — Electronic excitation with polarized light necessarily creates complementary orientational anisotropies from the excited and ground-state molecules. If the intermolecular interaction with the surrounding experienced by the excited-state molecules is different from that experienced by the ground-state molecules, a net excitation-induced orientational anisotropy will develop, enhancing the molecular reorientation provided directly by the optical field. This effect is analogous to that observed in dye-doped liquid crystals (LC) when dye molecules are excited. We report here the study of the effect in a pure isotropic LC medium. We use an optical pump-probe method to observe the excitation-induced reorientational dynamics. As the system relaxes back from picosecond pulse excitation, an increase in the orientational anisotropy of the ground-state molecules is observed, signifying the enhanced optical reorientation due to the state-dependent intermolecular interaction. The observed dynamics is well predicted by a mean-field model describing the intermolecular interaction between LC molecules. This work was supported by NSF

3:30PM W21.00006 Effect of disorder on a nematic-smectic A phase transition<sup>1</sup>, SIMON LAROCHELLE, MEHMET RAMAZANOGLU, Dept. of Physics, University of Toronto, ROBERT J. BIRGENEAU, Dept. of Physics, University of Toronto and Dept. of Physics, University of California Berkeley — Using X-ray scattering, we studied the nematic to smectic A phase transition of the liquid crystal butyloxybenzilideneoctylaniline (40.8) confined in an aerosil gel. The aerosil particles introduce quenched randomness in the system by providing pinning centers to the liquid crystal molecules. We find that the introduced disorder destroys the long range nature of the phase transition, and that the transition becomes similar to a transition in a finite-size system. Finite low temperature correlation lengths of the ordered moments are measured and the order parameter follows a power law behavior with respect to the reduced temperature in a limited temperature range. We also show evidence for a shift of the effective order parameter critical exponent  $\beta$  with increasing disorder.

<sup>1</sup>Work supported by NSERC Canada and U. S. DOE

#### 3:42PM W21.00007 Observation of polarization current accompanying smectic A electroclinic

**reorientation**, RENFAN SHAO, LIXING WANG, CHRISTOPHER D. JONES, DAVID A. COLEMAN, DUNG NGUYEN, MICHI NAKATA, JOSEPH E. MACLENNAN, LCMRC and Univ of Colorado, PER RUDQUIST, Chalmers Univ of Tech, DAVID M. WALBA, NOEL A. CLARK, LCMRC and Univ of Colorado — We have been studying the liquid crystalline material W530, and report observations of polarization current of the field-induced molecular reorientation in the SmA phase. W530 exhibits the following phase diagram on cooling: isotropic – SmA – uncharacterized Sm'X' – metastable SmC – crystal. The temperature range of the SmA and SmX phases is ~50°C, and ×-ray diffraction (XRD) shows very little layer spacing change throughout the width of these two phases, while the SmC fractional layer compression is ~5%. The SmX is nearly identical in appearance to the SmA phase under depolarized light microscopy (DPLM). However, when measuring polarization current while cooling from SmA to SmX, two polarization peaks appear throughout the range of the SmX phase. By adapting the Langevin model for deVries SmA, we are able to explain the two polarization peaks. Through a combination of DPLM cone angle and birefringence measurements, dielectric spectroscopy measurements, aligned sample and powder XRD experiments, and freely suspended film observations, we are able to show that the previously uncharacterized phase is a deVries SmA. Work supported by NSF MRSEC Grant DMR-0213918.

**3:54PM W21.00008 Defects in liquid crystal nematic shells**, A. FERNANDEZ-NIEVES, A.S. UTADA, V. VITELLI, D.R. LINK, D.R. NELSON, D.A. WEITZ, Harvard University — We generate water/liquid crystal (LC)/water double emulsions via recent micro-capillary fluidic devices [A. S. Utada, et.al. Science 308, 537 (2005)]. The resultant objects are stabilized against coalescence by using surfactants or adequate polymers; these also fix the boundary conditions for the director field n. We use 4-pentyl-4-cyanobiphenyl (5CB) and impose tangential boundary conditions at both water/LC interfaces by having polyvinyl alcohol (PVA) dispersed in the inner and outer water phases. We confirm recent predictions [D. R. Nelson, NanoLetters 2, 1125 (2002)] and find that four strength s=+1/2 defects are present; this is in contrast to the two s=+1 defect bipolar configuration observed for bulk spheres [A. Fernandez-Nieves, et.al. Phys. Rev. Lett. 92, 105503 (2004)]. However, these defects do not lie in the vertices of a tetrahedron but are pushed towards each other until certain equilibration distance is reached. In addition to the four defect shells, we observe shells with two s=+1 defects and even with three defects, a s=+1 and two s=+1/2. We argue these configurations arise from nematic bulk distortions that become important as the shell thickness increases. Finally, by adding a different surfactant, sodium dodecyl sulphate (SDS), to the outer phase, we can change the director boundary conditions at the outermost interface from parallel to homeotropic, to induce coalescing of the two pair of defects in the four defect shell configuration to yield two defect bipolar shells.

4:06PM W21.00009 Water as a Wetting Agent for Liquid Crystal Films, ERGYS SUBASHI, RAFAEL GARCIA, Worcester Polytechnic Institute — The dewetting of nCB liquid crystals from silicon wafer surfaces was first observed in 1999 [1] and has since grown into a subject of great fascination. The dewetting behavior occurs within a narrow coexistence region just below the nematic-to-isotropic phase transition temperature. When a wetted film is brought within this coexistence region, the film splits into two film thicknesses that are in apparent equilibrium with each other. A tentative but highly controversial explanation for this phase diagram has been proposed van Effenterre [2] in terms of mean field forces acting within the film. In our laboratory, we have undertaken a high-resolution measurement of the shape of this dewetting region for 5CB on silicon in search of evidence for the existence of fluctuation-induced forces that affect the thickness of these films. We have found, to our surprise, that ambient humidity affects the wetting behavior. Based on preliminary evidence taken thus far, water appears to act as a wetting agent that promotes the wetting of 5CB on silicon. We will present measurements showing how water affects the two-film thickness coexistence region. [1] F Vandenbrouck et al., Phys. Rev. Lett. 82, 2693 (1999). [2] D. Van Effenterre et al., Phys. Rev. Lett. 87, 125701 (2001).

#### 4:18PM W21.00010 Surface morphology of SiO deposited substrates and alignment of nematic

 $LC^{*_1}$ , LEELA JOSHI, SATYENDRA KUMAR, Department of Physics, Kent State University, Kent, OH 44242, RICCARDO BARBERI, Physics Department, University of Calabria, 87036 Rende (CS), Italy — Glass substrates with thin film of SiO are known to align nematic liquid crystals homogeneously for oblique deposition. X-ray reflectivity was employed to probe the surface morphology of approximately 150Å thick SiO films deposited at different landing angles. The interfacial roughness and morphological anisotropy was determined along the two orthogonal in-plane directions and the average electron density profile of the film calculated. The results show that the homogeneous and planar aligning films consists of SiO film with different roughness anisotropy and film thickness. The results will be discussed in light of previous reflectivity and AFM results on SiO [1] and other [2] surfaces. [1]. R. Barberi, Giocondo, G.V. Sayko, AK. Zvezdin, Phys. Lett. A213, 293 (1996). [2]. S. Kumar, J.-H. Kim, and Y. Shi, Phys. Rev. Lett. 94, 077803 (2005).

<sup>1</sup>\* Supported by the National Science Foundation grant DMR-03-12792.

4:30PM W21.00011 Crystal Nucleation behavior near gas-liquid spinodal line, LIMEI XU, Boston University, GIANCARLO FRANZESE, Universitat de Barcelona, SERGEY V. BULDYREV, Yeshiva University, H. E. STANLEY, Boston University — The complex problem of crystal nucleation is currently at stage. Using molecular dynamics simulations, we study the crystal nucleation behavior of colloids modeled by hard-core particles with narrow square well attractive potential. For this system the liquid gas critical point lies below the gas-crystal equilibrium line. We investigate how the nucleation rate depends on the pressure and density, in particular in the vicinity of the liquid-gas spinodal. We find that there is a correlation between nucleation rate and spinodal line. We interprete our results using classical nucleation theory.

#### 4:42PM W21.00012 Entropy driven formation of a chiral liquid crystalline phase of helical rods

, ZVONIMIR DOGIC, Rowland Institute at Harvard University, EDWARD BARRY, ZACH HENSEL, MICHAEL ŠHRIBAK, Marine Biological Laboratory, Woods Hole, RUDOLF OLDENBOURG, Marine Biological Laboratory, Woods Hole — We study the liquid crystalline phase behavior of a concentrated suspension of helical flagella isolated from Salmonella typhimurium. With increasing concentration, a suspension of helical flagella undergo an entropy driven first order phase transition to a liquid crystalline state having a novel chiral symmetry. Flagella are prepared with different polymorphic states, some of which have a pronounced helical character while others assume a rod-like shape. We show that the static phase behavior and dynamics of chiral helices are very different when compared to simpler achiral hard rods. 4:54PM W21.00013 Dynamics of Director Fluctuations in Confined and Filled Liquid Crystals. , EDWIN ARROYO, SARMISTHA BASU, FOUAD ALIEV, University of Puerto Rico — Dynamic light scattering was applied to study the influence of randomness as well of boundary conditions (planar-axial and homeotropic-radial) and layer thickness (at nanoscale) of 5CB and 8CB confined to random porous matrices, to cylindrical pores and filled with Aerosil particles (hydrophilic and hydrophobic) on phase transitions and relaxation of director orientational fluctuations. For confined 8CB in the nematic phase two well-defined relaxation processes were for confined liquid crystals. The first process is associated with bulk-like nematic director fluctuations. The second relaxation process (with relaxation time slower than the first one) is most likely due to the fluctuations in layers nearest the wall surface. We found that for homeotropic boundary conditions of confined liquid crystal, the pore wall-liquid crystal interactions influence on the properties of the surface layer is stronger than in the case of axial orientation, particularly, and the influence of boundary conditions on N-Sm-A phase transition in confined 8CB is stronger than on isotropic- nematic phase transition. The separation between the first and the second (slow) process is clearer for thinner layers and the amplitude of slow process is greater for thinner layers. This suggests that the slow process is surface relaxation. This relaxation was observed in filled liquid crystals as well.

5:06PM W21.00014 Micro-focus synhrotron X-ray diffraction study of novel mesomorphic porphyrin derivatives<sup>1</sup>, SHIN-WOONG KANG, LANFANG LI, QUAN LI, Kent State University, Kent, OH 44242, MICHI NAKATA, University of Colorado, Boulder, CO 80309, BRANDON CHAPMAN, RONALD PINDAK, Brookhaven National Laboratory, Upton, NY 11973, SATYENDRA KUMAR, National Science Foundation, 4201 Wilson Blvd., Arlington, VA 22230 — The mesophase structures of three novel mesomorphic porphyrin derivatives were examined using polarized optical microscopy and microfocus synchrotron X-ray diffraction at various temperatures using a beam with a 14  $\mu$ m×14 $\mu$ m cross-section at the bending magnet beamline of Sector 20 at the Advanced Photon Source. The x-rays were diffracted from microscopic monodomains in thin glass cells while simultaneously observing the optical textures. The results confirmed a hexagonal arrangement of discotic columns in the liquid crystalline phase. At a lower temperature, highly ordered plastic crystal phase was obtained. The results of the microdiffraction experiment and promising properties of these compounds as a carrier transporting material will be presented.

<sup>1</sup>Supported by the National Science Foundation grant DMR-0312793.

5:18PM W21.00015 Stochastic Rotation Dynamics: generalizations and applications for nonideal fluids, binary mixtures and colloids, THOMAS IHLE, Department of Physics, North Dakota State University, ERKAN TUZEL, School of Physics and Astronomy, University of Minnesota, DANIEL KROLL, Department of Physics, North Dakota State University — A particle-based algorithm for the coarse-grained modeling of a fluctuating Solvent, namely Stochastic Rotation Dynamics (SRD), was recently introduced by Malevanets and Kapral[1]. This algorithm describes a fluid with an ideal gas equation of state and has been successfully applied to study polymers, colloids, and vesicles in flow. Here, we present generalizations of SRD for modeling fluids with non-trivial equations of state[2]. In particular, we show how to model a simple liquid with a non-ideal equation of state by incorporating excluded volume effects. We show the thermodynamic consistency of the model by independently measuring the pressure, density fluctuations and the speed of sound and compare with analytical results. This idea is extended to model binary mixtures with a miscibility gap; and the phase diagram of such a mixture will be presented. Furthermore, colloids are included in the SRD solvent and results for colloidal suspensions driven by external forces will be shown. [1] A. Malevanets, R. Kapral, J. Chem. Phys. 110, 8605 (1999). [2] T. Ihle, E. Tuzel, D. M. Kroll, cond-mat/0509631.

#### Thursday, March 16, 2006 2:30PM - 5:30PM -

Session W33 DFD: Nonequilibrium and Templated Assembly Baltimore Convention Center 336

2:30PM W33.00001 Designing elastic sheets to self-assemble in a viscous environment, SILAS ALBEN, MICHAEL BRENNER, Harvard University — A recent work by Boncheva et al. (Proc. Nat. Acad. Sci. 2005 102: 3924-3929) has raised some basic issues about designable self-assembly within the context of planar elastic sheets which fold into 3D structures under magnetic forces. While being agitated in water, millimeter-scale structures were shown to fold with varying success depending on the locations of magnets on the sheets. Our work considers how to design such structures, an understanding of which will be necessary when moving this process to the micron scale. Among the important parameters are the geometry of the flat sheet, the configurations of the magnets, and the ratios of magnetic to elastic forces. We consider this problem using a numerical model of an elastic sheet, and restrict to the simpler case of electrostatic forces in a quasi-static limit. We identify a simple algorithm for choosing configurations of a sphere and more general geometries, in the overdamped viscous regime. We also give an asymptotic formula for the elastic energy in the thin-plate limit.

#### 2:42PM W33.00002 Dynamic self-assembly of magnetic particles on the fluid interface: surface

wave assisted effective magnetic exchange, ALEXEY SNEZHKO, IGOR ARANSON, WAI-KWONG KWOK, Materials Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439 — Novel dynamic self-assembled multi-segment magnetic structures ("snakes") induced by a vertical alternating magnetic field in an ensemble of magnetic particles suspended on a liquid/air interface are reported. We demonstrate that these structures are directly related to surface waves in the liquid generated by the collective response of magnetic microparticles to the alternating magnetic field. The segments of magnetic "snake" exhibit long-range antiferromagnetic ordering mediated by the surface waves, while each segment is composed of ferromagnetically aligned chains of microparticles. To describe observed magnetic behavior of the generated structures we propose a simple phenomenological model where the effect of surface waves is replaced by an effective exchange interaction. In the framework of the proposed model the effective exchange constants corresponding to different regimes of magnetic driving were extracted from the experimental data.

#### 2:54PM W33.00003 Demonstration of shape selectivity in depletion-induced colloidal aggre-

**gation**, STEPHANE BADAIRE, JOSEPH W. WOODY, CECILE COTTIN-BIZONNE, ABRAHAM D. STROOCK, Dept of Chemical and Biomolecular Engineering - Cornell University — We have developed a set of monodisperse, non-spherical colloids using photolithography in order to elucidate fundamental questions related to the role of shape in defining colloidal phase behaviour and, eventually, to build new microstructured materials. Our goal is to use depletion and DLVO forces to induce specific and directional interactions during the aggregation process of these non-spherical colloids. We will first describe the development and basic characterization of these particles, including index of refraction, zeta potential, polydispersity, and surface roughness. We will then present an initial state diagram of depletion-induced structure, and provide mechanistic insight into the role of specific characteristics of the particles in defining this behaviour. We will finally discuss theoretical calculations of the expected interactions and the possibility of generalizing the results to other colloidal systems.

#### 3:06PM W33.00004 Pattern formation and liquid crystallinity in evaporating drops of gold

**nanorods.**, KYOUNGWEON PARK, VIVEK SHARMA, School of Polymer, Textile and Fiber Engineering, MOHAN SRINIVASARAO, School of Polymer, Textile and Fiber Engineering and School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA — The drying drops of colloidal rods on glass provide a coffee ring type stain accompanied by formation of highly birefringent deposit, suggesting lyotropic liquid crystalline phase forms prior to deposit formation. Further, Liesegang ring like patterns which have concentric deposits, appear on drying, only under specific conditions, and in optical microscope show similar birefringent bands. Similar experiments done on carbon coated copper TEM grids and observed under TEM, show smectic and nematic-like phases as well as create vortex-like assembly of nanorods reminiscent of defect structures in liquid crystals, and are likewise explained in terms of lowest energy configuration of twist configuration. In the present, work we compliment the rich experimental observations, by proposing mechanisms that explain formation of concentric rings, as well as other complex patterns using both the existing framework based on coffee ring stain models and on basis the observed liquid crystalline phase behavior.

**3:18PM W33.00005 Molecular Detection with Self-Assembled Gold Nanoparticle Wires**, J.B. HUTCHISON, George Washington University, J.A. HOFFMANN, George Washington University, J.W. SUN, George Washington University, M.E. REEVES, George Washington University — Recently, we have reported the creation of gold nanowires by evaporation-driven vertical colloidal deposition (VCD) of gold nanoparticles. Subsequently, we have noted systematic changes in conductivity associated with post-deposition annealing. Here we describe the change in room temperature conductivity of gold nanoparticle wires after exposure to thiol-derivatized molecules. A self-assembled gold nanoparticle wire is immersed into a solution of octadecanethiol (ODT) dissolved in ethanol. An ODT molecule comprises a sulfur atom and a short hydrocarbon chain. The sulfur atoms form metallic bonds with the conduction electrons on the surface of the gold nanoparticles, and the high surface to volume ratio of the wire allows us to see a marked jump in resistance. We have seen roughly a 10 percent increase in the resistance of previously annealed wires when immersed in 2 millimolar ODT solution. Further experiments include measurement of resistance as a function of thiol-concentration and as a function of wire preparation prior to immersion.

3:30PM W33.00006 Orientational Order of Molecular Assemblies on Inorganic Crystals<sup>1</sup>, JAEHUN CHUN, Department of Chemical Engineering, Princeton University, DUDLEY SAVILLE, Department of Chemical Engineering, Princeton University, JE-LUEN LI, Department of Chemistry, Princeton University, HANNES SCHNIEPP, Department of Chemical Engineering, Princeton University, ROBERTO CAR, Department of Chemistry, Princeton University, ILHAN AKSAY, Department of Chemical Engineering, Princeton University – Surfactant micelles form oriented arrays on crystalline substrates such as HOPG (Highly Ordered Pyrolytic Graphite) although registration is unexpected since the template unit cell is small compared to the size of a rod-like micelle. In addition, with atomic force microscopy, we show that orientational ordering is a dynamic, multi-molecule process. Interaction energy calculations based on molecular simulations reveal that orientational energy differences on a molecular scale are too small to explain matters. However, treating the cooperative processes as a balance between van der Waals torque on a large, rod-like micellar assembly and Brownian motion shows that orientation is favored. Our study provides a physical insight on regulation of self-assembly structures at small length scale.

<sup>1</sup>The NASA University Research, Engineering, and Technology Institute on BioInspired Materials (BIMat) under Award No. NCC-1-02037 and the National Science Foundation (MRSEC program) through the Princeton Center for Complex Materials (DMR 0213706)

3:42PM W33.00007 Vesicle-Templated Supramolecular Assembly of Alginate Nanogels, JENNIFER HONG, National Institutes of Standards and Technology NIST/University of Maryland College Park, WYATT VREELAND, NIST, Analytical Chemistry Division CSTL, SRINIVASA RAGHAVAN, University of Maryland College Park. Department of Chemical & Biomolecular Engineering, LAURIE LOCASCIO, NIST, Analytical Chemistry Division CSTL, MICHAEL GAITAN, NIST, Semiconductor Electronics Division EEEL — In this work, large uni- and multilamellar dipalmitoyl phosphatidylcholine (DPPC) liposomes (800-900 nm in diameter) were used as templates for the formation of alginate gels. DPPC liposomes encapsulating sodium alginate were prepared in a 15 mM NaCl buffer solution by the solvent injection method, followed by several freeze/thaw cycles to achieve higher encapsulation efficiency and larger vesicle size. Purified liposomes were placed in a 10 mM CaCl2 buffer solution and permeabilized by heating and cooling over the phase transition temperature (Tm) of DPPC. The increased membrane permeability at the Tm allowed calcium ions from the surrounding buffer solution to traverse the membrane to the interior region and subsequently crosslink the encapsulated alginate. Removal of the lipid by detergent resulted in nanogels that were similar in size (800-900 nm in diameter) to the template liposome, as characterized by multi-angle and dynamic light scattering techniques. In the future these nanogels may be useful for single-molecule encapsulation or controlled release applications.

#### 3:54PM W33.00008 Self-Assembly of Two Dimensional Hard Rod Fluids in the Presence of

Surface Barriers, DEREK A. TRIPLETT, KRISTEN A. FICHTHORN, The Pennsylvania State University — Hard rods are interesting building blocks for assembly as they organize themselves into different phases depending on their aspect ratio and concentration. Much work has been done to develop an understanding of the various phases exhibited by bulk, hard-rod fluids in two and three dimensions. For applications in nanoelectronics, it is desirable to be able to assemble nanowires into various structures conducive to nanocircuitry. In this work, we use Monte Carlo simulations to examine the phase behavior of two different systems involving two-dimensional, colloidal nanowires. In the first study, we probe the influence of regularly spaced surface barriers on the ordering of two-dimensional hard rods. By varying the spacing between the barriers and their size relative to the rods, we demonstrate that a number of interesting phases can be achieved, indicating that surface barriers can effectively tune the alignment of the rods. In a second study, we probe the hard-sphere templated assembly of colloidal nanowires. We demonstrate that a number of interesting and potentially beneficial phases occur as the rod length relative to the sphere diameter, rod aspect ratio, and concentration is varied.

4:06PM W33.00009 Multipolar interaction model for microtubule self-assembly<sup>1</sup>, KYLE GUSTAFSON, Univ. of MD, Dept. of Physics, IREAP, JUSTIN STAMBAUGH, MIT Lincoln Lab., WOLFGANG LOSERT, Univ. of MD, Dept. of Physics, IPST and IREAP — Tubulin protein monomers (m = 50 kDa, d = 4-5 nm) are known to self-assemble into biologically significant structures called microtubules. Calculations for microtubule models using the full crystallographic structure of tubulin are prohibitive. As a substitute, we investigate a simpler multipolar interaction model of tubulin which can capture important features of microtubules. We present energy-minimization calculations showing that a four point-charge rectangular model reproduces the 0.93 nm staggering of observed microtubules. We then attempt to validate these static Coulomb calculations with molecular dynamics (MD) using NAMD (from the Theoretical and Computational Biophysics group at the University of Illinois). These simulations include electrostatic interactions, stiff bonded interactions, a Lennard-Jones potential and Langevin damping. The results of the MD simulations are strongly dependent on each of these influences. We find stable filaments of tubulin using the multipole model in MD simulations. When these filaments are combined into a realistic microtubule in MD, an energy minimum is found which supports a stable tube. The study encompasses fraying of tube ends, staggering angle, and ring stability for tubulin and microtubules based on our simple, four charge multipolar model.

<sup>1</sup>The primary author is supported by a Fannie and John Hertz Foundation Graduate Fellowship.

4:18PM W33.00010 Thermoreversible Vesicle-to-Micelle Transitions in Surfactant-Salt Mixtures, AIMEE KETNER, TANNER DAVIES, SRINIVASA RAGHAVAN, Department of Chemical and Biomolecular Engineering, University of Maryland, College Park, MD 20742 — Mixtures of the cationic surfactant, CTAB and the organic compound, 5-methyl salicylic acid (5mS) spontaneously self-assemble into unilamellar vesicles at room temperature. Upon heating, these vesicles undergo a thermoreversible transition to wormlike micelles. This phase transition results in a 1000-fold increase in the solution viscosity with increasing temperature. Small-angle neutron scattering (SANS) measurements show that the phase transition from vesicles to micelles is a continuous one, with the vesicles and micelles co-existing over a range of temperatures. A mechanism for the above phase transition is proposed, based on the desorption of bound aromatic counterions from the vesicle as a function of temperature. **4:30PM W33.00011 Self-assembly models for lipid mixtures**, DIVYA SINGH, Johns Hopkins University, LIONEL PORCAR, NIST Center for Neutron Research, PAUL BUTLER, NIST Center for Neutron Research, URSULA PEREZ-SALAS, UC, Irvine — Solutions of mixed long and short (detergent-like) phospholipids referred to as "bicelle" mixtures in the literature, are known to form a variety of different morphologies based on their total lipid composition and temperature in a complex phase diagram. Some of these morphologies have been found to orient in a magnetic field, and consequently bicelle mixtures are widely used to study the structure of soluble as well as membrane embedded proteins using NMR. In this work, we report on the low temperature phase of the DMPC and DHPC bicelle mixture, where there is agreement on the discoid structures but where molecular packing models are still being contested. The most widely accepted packing arrangement, first proposed by Vold and Prosser had the lipids completely segregated in the disk: DHPC in the rim and DMPC in the disk. Using data from small angle neutron scattering (SANS) experiments, we show how radius of the planar domain of the disks is governed by the effective molar ratio  $q_{eff}$  of lipids in aggregate and not the molar ratio q(q = [DMPC]/[DHPC] as has been understood previously. We propose a new quantitative (packing) model and show that in this self assembly scheme,  $q_{eff}$  is the real determinant of disk sizes. Based on  $q_{eff}$ , a master equation can then scale the radii of disks from mixtures with varying q and total lipid concentration.

4:42PM W33.00012 End-to-End Adhesion of Short Duplex DNA Oligomers , TOMMASO BELLINI, University of Milano, Italy, NOEL CLARK, University of Colorado — The classic model for the formation of liquid crystal phases of rod shaped objects was presented by Onsager, who showed that hard rods of length L and diameter D form a nematic phase when volume fraction is f > fc = 4D/L. This criterion is obeyed reasonably well for rod-shaped nucleosomal [150 base pair (bp)] B-DNA duplexes (L = 50nm, D = 2nm). Recently we found, however, that very short duplex B-DNA oligomers, 6bp – 20bp (2 to 6nm) in length, form similar nematic and columnar LC phases, even though their L/D ratio is almost 1 and f << fc. We attribute these phases to intermolecular interaction which provides an end-to-end adhesion force between these short oligomers to form extended anisotropic "living polymers." The theory of the formation of such anisotropic aggregates will be reviewed and applied to the DNA observations. Work supported by NSF MRSEC Grant DMR 0213918 and NSF Grant 0072989.

4:54PM W33.00013 Modeling of fractal intermediates in the self-assembly of silicatein filaments<sup>1</sup>, MEREDITH MURR, UCSB, GUNJAN THAKUR, UCSB, IGOR MEZIC, UCSB, DANIEL MORSE, UCSB — Silicateins are proteins with catalytic, structure-directing activity that are responsible for silica biosynthesis in certain sponges, Self-assembly of the silicatein monomers and oligomers was previously shown experimentally (Murr and Morse 2005) to form fibrous structures through the formation of diffusion limited, fractally patterned aggregates on the path to filament formation. We present a diffusion-limited aggregation (DLA) based model that is capable of capturing the basic properties of this self-assembly process. The Silicatein oligomer is modeled with three sites of attachment. Rules of attachment are specified that allow for specific interaction between these sites when oligomers are in proximity. The process differs from a DLA process in the following: 1) The process of aggregation is continued dynamically, i.e. the growing structures are spatially distributed and keep diffusing as they are growing 2) The molecules are oriented. Thus rotational diffusion is important. 3) The attachment can happen at more than 1 site and the strength of the active sites can be varied. We show that the self-assembled structures have a good level of similarity with the in-vitro experimental results. We quantify this by comparing the fractal dimension of the experimental data and the model output.

<sup>1</sup>Partially funded by the Institute for Collaborative Technologies, UCSB.

5:06PM W33.00014 Structure of Porous Columns Self-assembled from Dendritic Dipeptides<sup>1</sup>, PAUL HEINEY, MIHAI PETERCA, VENKAT BALAGURUSAMY, Physics Dept., Univ. of Pennsylvania, STEVEN HUDSON, National Inst. of Standards and Technology, ANDRES DULCEY, VIRGIL PERCEC, Dept. of Chemistry, Univ. of Pennsylvania — Synthetic pores are an important step in the development of biomimetic materials incorporating features such as trans-membrane channels, gene delivery, protein folding, and selective encapsulation. We have used small-angle xray scattering to study helical pores self-assembled from dendritic dipeptides. The main features of the supramolecular assembly are computed by least-squares fitting the parameters of a simplified structural model to the x-ray diffraction data. This work reports the supramolecular assembly temperature stability and conformational changes of the 3-dimensional packing as a function of dipeptide structure and stereochemistry. The results provide a methodology to design the synthetic pores in order to control the pore size and separation at the Å level, according to the desired function.

<sup>1</sup>Supported by the MRSEC program of the National Science Foundation under award DMR05-20020.

5:18PM W33.00015 X-ray Study of the Electrical Double Layer at the Oil - Water Interface<sup>1</sup>, ALEKSEY TIKHONOV, CARS-The University of Chicago — Our understanding of the structure of the insulator/electrolyte solution interface is of fundamental

importance in describing electrochemical processes in systems involving membranes, absorbers, catalysts, surfactants, or surfaces of other dielectrics. Due to the specific interaction of the solvent with the insulator, a heterogeneous highly polarized region or an electrical double layer forms at the boundary between bulk phases. We studied the spatial structure of the transition region between n-hexane (insulator) and silica sol (electrolyte) solution by x-ray scattering. The structure factor of the interface and the angular dependence of the grazing incidence small-angle scattering can be explained by the interfacial model, which agrees with the theory of the electrical double layer, shows the separation of positive and negative charge, and consists of three layers, i.e., a thin layer of Na<sup>+</sup>, a monolayer of nanocolloidal particles as the part of the diffuse layer, and a low-density layer sandwiched between them.

<sup>1</sup>Brookhaven National Laboratory is supported by U.S.D.O.E., Contract No. DEAC0298CH10886. X19C is partially supported through funding from the ChemMatCARS National Synchrotron Resource and the University of Chicago.

## Thursday, March 16, 2006 2:30PM - 5:30PM -

Session W34 DFD: Fluid Structure & Properties Baltimore Convention Center 337

#### 2:30PM W34.00001 Scaling fields and the nature of liquid-gas asymmetry in fluids, JINGTAO WANG,

University of Maryland, CLAUDIO CERDEIRIÑA, Universidad de Vigo, Spain, MIKHAIL ANISIMOV, JAN SENGERS, University of Maryland — Fisher and coworkers [Phys. Rev. Lett. **85**, 696 (2000); Phys. Rev. E **67**, 061506 (2003).] recently suggested that in fluids the two theoretical scaling fields, commonly known as "ordering" and "thermal", are mixtures of three physical fields, namely, chemical potential, temperature, and pressure. We have examined experimental consequences of this formulation ("complete scaling") with regard to the asymmetry of vapor-liquid coexistence in real fluids. By analyzing the coexisting curves of various fluids, we have shown that the vapor-liquid asymmetry originates from two different sources: one from mixing of chemical potential and pressure into the thermal field and another one from mixing of pressure into the ordering field. The first source is attributed to a correlation between entropy and density, whereas the second source is associated with the excluded volume. Real fluids can be mapped into the symmetric lattice-gas (lsing-like) model by a redefinition of the order parameter that can be now expressed through a combination of density, entropy, and molar volume. We have also demonstrated which molecular parameters of fluids control these two sources of vapor-liquid asymmetry.

#### 2:42PM W34.00002 NMR characterization of complex fluids by diffusion – relaxation distrib-

**ution functions** , MARTIN HURLIMANN, Schlumberger - Doll Research, ALBINA MUTINA, Kazan State University, Russia — Many natural fluids are complex mixtures of different types of molecules. As an example, the molecular composition of crude oils typically consists of molecules with a number of carbon atoms that range between one to over 100. In addition to the diverse size, the constituent molecules can be classified into different chemical classes, such as saturates, aromatics, resins and asphaltenes. It is well known that measurements of diffusion and NMR relaxation times can give information on molecular size. We demonstrate that two-dimensional diffusion – relaxation time distribution functions, f(D,T2), can provide a more unique fingerprint of complex fluids with information on both chain length distribution and chemical composition. The new approach is illustrated with results for different crude oils. The experiments were conducted at a Larmor frequency of 5 MHz and temperatures between 10 C and 58 C. The measurements show a strong correlation between the distribution sof diffusion coefficients and relaxation times that are sample specific. The diffusion – relaxation function provides information on the correlation between the rotational and the translational diffusion coefficients of each component of the fluid.

2:54PM W34.00003 Structural Change of the Mixtures of Ionic Liquid and Water Studied by Infrared Absorption Spectroscopy, DOSEOK KIM, YOONNAM JEON, JAEHO SUNG, Department of Physics and Interdisciplinary Program of Integrated Biotechnology, Sogang University, Seoul 121-742 Korea, YUKIO OUCHI, Department of Chemistry, Nagoya University, Chikusa-ku, Nagoya 464-8602 Japan — Infrared absorption spectra of the mixtures of ionic liquid and water (1-butyl-3-methylimidazolium tetrafluoroborate, [BMIM]BF<sub>4</sub>) with varying concentrations were obtained by Attenuated Total Reflection (ATR) method. Investigation of the spectra in the OH-stretch vibration range indicated the structural change of the water with the change in the concentration. At very low concentration of water, two peaks around  $3600cm^{-1}$  were assigned to the monomeric form of water molecules weakly hydrogen bonded to the BF<sub>4</sub><sup>-</sup> anions. With the increase in the water concentration, the broad feature at ~3460cm<sup>-1</sup> corresponding to the bulk water took over the above monomeric peaks, which gradually redshifted with the increased water concentration. In the range from 2800 to  $3200cm^{-1}$  for the various CH-stretch vibration modes in the cation, the peaks in this ranged blueshifted with the increase in the water concentration. This blueshift was as much as ~7cm<sup>-1</sup> for the CH<sub>3</sub> vibration modes of butyl chain while it hardly changed for the modes for the CH attached to the imidazolium core, suggesting varying degree of interactions between the carbon-bonded hydrogen and the water molecules.

**3:06PM W34.00004 Weighted density functional theory for water**, SAHAK PETROSYAN, DAVID ROUNDY, JEAN-FRANCOIS BRIERE, TOMÁS ARIAS, Cornell University — We report a weighted density functional theory for water that correctly describes bulk properties of water as well as perturbations at large and small length scales. Calculation of the free energy of solvation for hard sphere solutes of different sizes verifies that this functional gives a simple description of the hydrophobic effects in water. Use of this functional within a joint-density functional theory framework allows a rigorous replacement of molecular water with a continuum in Kohn-Sham calculations of systems in equilibrium with a solution.

3:18PM W34.00005 Small-angle neutron scattering study of pH dependence of the liquid structure factor of concentrated solutions of eye lens gamma-B crystallin, KENNETH DESMOND, GEORGE THURSTON, Department of Physics, Rochester Institute of Technology, ANNA STRADNER, PETER SCHURTENBERGER, Department of Physics, U. Fribourg — We are evaluating the pH dependence of the liquid structure of aqueous solutions of the eye lens protein, gammaB crystallin, near its critical point for liquid-liquid phase separation, to help evaluate the influence of protein charge on the phase separation. We have obtained small-angle neutron scattering data from gammaB crystallin solutions at pH 6.4, 7.1 and 7.4 in a 0.1 M sodium phosphate buffer, and at pH 4.5 in a 0.020M sodium acetate buffer, all in D20. Protein concentrations ranged from 6 to 260 mg protein/ml solution and the scattering vector magnitude (q) ranged from 0.004 to 0.45 inverse Angstroms. At pH 6.4 to 7.4 liquid structure factors vs. concentration and temperature near the cloud point for liquid-liquid phase separation are well represented, in general, by the Baxter sticky sphere model. In contrast, at pH 4.5, concentrated gammaB shows a very different liquid structure indicating highly repulsive interprotein interactions, consistent with both high net protein charge and reduced screening.

3:30PM W34.00006 Phase behavior and mixing-demixing transitions in binary liquid mixtures with spherical and non-spherical interactions<sup>1</sup>, ENRIQUE DIAZ-HERRERA, Depto. de Fisica, UAM-I (MEXICO), GUILLERMO RAMIREZ-SANTIAGO, Instituto de Fisica, UNAM (MEXICO), J. ANTONIO MORENO-RAZO, Depto. de Fisica, UAM-I (MEXICO) — We have carried out extensive equilibrium molecular dynamics simulations to study the temperature versus density phase diagrams and the mixing-demixing transition line in fluid equimolar binary mixtures modeled by: (i) Lennard-Jones, (ii) Stock-Mayer, and (iii) Gay- Berne molecular interactions. These studies are performed as function of miscibility parameter,  $\alpha = \epsilon_{AB}/\epsilon_{AA}$ , where  $\epsilon_{AA} = \epsilon_{BB}$  and  $\epsilon_{AB}$  stand for the parameters related to the attractive part of the intermolecular interactions for similar and dissimilar particles, respectively. When the miscibility of the Lennard-Jones mixture varies in the range  $0 < \alpha < 1$ , a continuous critical line of consolute points  $T_{cons}(\rho)$ , appears. This line intersects the liquid-vapor coexistence curve at different positions depending on the values of  $\alpha$ , yielding mainly three different topologies for the phase diagrams. These results are in qualitative agreement to those found previously for square well and hard-core Yukawa binary mixtures. We also carry out a detailed study of the liquid-liquid interfacial and liquid-vapor surface tensions, as function of temperature and miscibility as well as its relationship to the topologies of the phase diagrams. Similar studies and analysis are also performed for Stock-Mayer and Gay-Berne binary mixtures.

<sup>1</sup>Supported by DGAPA-UNAM IN110103 & CONACYT 43596-F

3:42PM W34.00007 Confined Fluids: the Time Variable in the Force-Distance Profile , JANET WONG, SUNG-CHUL BAE, STEVE GRANICK, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign — Hithertooverlooked time dependence is known to play a prominent role in determining the friction of confined fluids. In this study, for the first time we introduce the time variable into measuring force-distance profiles of several simple alkane fluids. The existence of near-surface layered structures in confined fluids is generally manifested as oscillatory forces in force-distance profiles obtained using surface forces apparatus (SFA) and atomic force miscroscopy (AFM) experiments. While it is generally agreed that the rate of the experiment should be slow enough to achieve a quasi-static state, it is less clear what the appropriate rate should be. In this study, while maintaining the experimental time scale uniformly slow enough to avoid trivial hydrodyanamically-induced surface deformations, we demonstrate time dependence in the measured force-distance profile. The role of time scale on the actual structure of the confined fluid will be discussed.

#### 3:54PM W34.00008 Spectroscopic Observation of Fluid Molecular Alignment in a Molecularly-

Thin Confined Geometry , MINSU KIM, SHAN JIANG, SUNG CHUL BAE, STEVE GRANICK, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign — For the first time, we present data of molecular alignment of a linear chain (1,3-dicyanopropane) under confinement. Confinement was produced between two mica surfaces within a surface forces apparatus (SFA) and measurements employed confocal Raman spectroscopy. We focused on the  $CH_2$  symmetric stretch vibrations and CN triple bond stretch vibrations. A polar plot of Raman band intensity as a function of incident light polarization allows us to determine the orientation and order parameter of alignment. It is confirmed that alignment can be achieved discussed.

4:06PM W34.00009 Active Microrheology of Dense Colloidal Suspensions , ALEXANDER MEYER, ERIC M. FURST, Department of Chemical Engineering, University of Delaware — We investigate the active microrheology of a colloidal suspension using laser tweezers. The experimental system described here is composed of a hard sphere suspension of fluorescent, index-matched poly(methyl methacrylate) particles seeded with a low concentration of index-mismatched melamine probes. The probe particles are held in an optical trap and subjected to a uniform flow, enabling measurements of the suspension microrheology. Additionally, confocal microscopy is used to obtain non-equilibrium microstructural information. An anisotropic pair distribution function, with a dense region at the leading surface of the probe and a wake trailing it, is observed as the Péclet number increases to much greater than unity. This structural transition gives rise to a 49, 1483-1502 (2005)], and demonstrate the non-linear microrheology of colloidal suspensions.

#### 4:18PM W34.00010 Nonlinear microrheology of wormlike micelle solutions using magnetic

**nanowire probes**, NATHAN CAPPALLO, CLAYTON LAPOINTE, ROBERT L. LEHENY, DANIEL H. REICH, Johns Hopkins University — Using ferromagnetic Ni nanowires we investigate the local mechanical properties of wormlike micelle solutions composed of equimolar concentrations of the surfactant cetylpyridinium chloride (CPCI) and sodium salicylate (NaSal). Rotating the nanowires with external magnetic fields, we access both linear and nonlinear regimes of the fluid's rheology. The linear viscosity at low rotation rates is strongly temperature dependent as expected from mechanical rheometry experiments. At high rotation rates the viscosity exhibits pronounced shear thinning that is independent of temperature. The onset of the nonlinear regimes coincides with a transient, anisotropic shear-induced state in the fluid that generates a torque on the wire, causing it to tip out of the plane of rotation when the field is removed.

4:30PM W34.00011 Myelin figures: an Elastic Instability? , LING-NAN ZOU, SIDNEY R. NAGEL, The James Franck Institute, the University of Chicago — Myelin figures form when certain lamellar phase surfactants swell upon exposure to water. The formation of these myelins, which are tubular structures composed of multiple bilayers of surfactant, is puzzling because it represents the formation of a higher bending-energy configuration from a lower bending-energy initial state. We show that single myelins can be produced in isolation and require a driving force to form and grow; they retract into their parent structure when the driving is removed. We present a model, consistent with our experimental observations, where the formation of myelins is due to an elastic instability of the lamellar phase under internal stress. We propose an experiment to test of this model in comparison to other models, such as that of Huang et al.[1]

[1]J.-R. Huang, L.-N. Zou, and T. A. Witten, Eur. Phys. J. E (2005). DOI: 10.1140/epje/e2005-00035-8.

4:42PM W34.00012 Charge fluctuations and correlations in finite electrolytes , YOUNG C. KIM, Laboratory of Chemical Physics, NIDDK, NIH, Bethesda, 20892, MICHAEL E. FISHER, Institute for Physical Science and Technology, University of Maryland, College Park, 20742 — Charge fluctuations,  $\langle Q_{\Lambda}^2 \rangle$ , for the 1:1 equisize hard-sphere electrolyte with the diameter a are computed via grand canonical Monte Carlo simulations, where  $Q_{\Lambda}$  is the total charge inside a subvolume  $\Lambda$  contained in a simulation box of dimensions  $L \times L \times L$  with periodic boundary conditions. The charge fluctuations increase like the surface area  $|\partial\Lambda|$  as  $\Lambda$  increases, even for small system sizes  $L \leq 12a$ . For slabs of dimensions  $L \times L \times \lambda L$  with  $0 < \lambda < 1$ , the scaled charge fluctuations,  $\langle Q_{\Lambda}^2 \rangle / |\partial\Lambda|$ , approach the thermodynamic limits exponentially fast. The extrapolations to  $L \to \infty$  then yield the Lebowitz length,  $\xi_{L}(T,\rho)$ , where densities  $\rho \leq 3\rho_c$  and temperatures  $T \gtrsim T_c$  have been studied. An exact asymptotic expression is obtained for  $\langle Q_{\Lambda}^2 \rangle$ . This enables one to compute the charge correlation length  $\xi_Z(T,\rho)$  precisely. The results for  $\xi_Z(T,\rho)$  agree with Debye-Hückel-type theories at low densities, but show deviations as the density increases. Charge oscillations at higher densities are also observed, as anticipated theoretically. [1] Y. C. Kim, E. Luijten, and M. E. Fisher, Phys. Rev. Lett. **95**, 145701 (2005).

#### 4:54PM W34.00013 Solid or Liquid ? – Kinetically induced solidification in a simple nanocon-

**fined liquid**<sup>1</sup>, PETER HOFFMANN, Wayne State University, GEORGE MATEI, Wayne State University, SHIVPRASAD PATIL, Wayne State University, AHMET ORAL, Bilkent University — For many years there has been a controversy regarding the supposed solidification of simple liquids when they are confined to a few nanometer film thickness. By using a novel, ultra-small amplitude Atomic Force Microscopy (AFM) technique, we have found that solidification in these systems seems to be due to a kinetic effect and does not occur in thermodynamic equilibrium. In particular, we studied OMCTS confined between a flat silicon surface and a silicon tip and found that at very low approach speeds ( $\leq 0.3$  Å/sec) the confined fluid remains liquid-like with no change in mechanical relaxation time from the bulk, although ordering is observed in the stiffness and damping of the film. However, when approaching the tip slightly faster at or above 6 Å/sec, the liquid suddenly changes properties dramatically. In the ordered regime, damping is greatly reduced and the mechanical relaxation times show large peaks, indicating an elastic, solid-like response. This result suggests that the observed solidification is a non-equilibrium effect induced at very long time scales.

<sup>1</sup>Funding is acknowledged from NSF-MRI and NSF-CAREER

## 5:06PM W34.00014 Investigation of Liquid Transport/Diffusion through a Nanopore Driven by a Constant Pressure/Chemical Potential Difference., CUNKUI HUANG, University of Alberta, KUMAR NANDAKUMAR,

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#### 5:18PM W34.00015 Phase behavior in binary fluid mixtures with spherical and non-spherical

**interactions**, ENRIQUE DIAZ-HERRERA, Universidad Autonoma Metropolitana (Mexico), GUILLERMO RAMIREZ-SANTIAGO, Instituto de Fisica, UNAM (Mexico), J. ANTONIO MORENO-RAZO, Universidad Autonoma Metropolitana (Mexico) — We have carried out extensive MD simulations to study the T vs.  $\rho$  phase diagram and the mix-demix transition in fluid binary mixtures with (1) Lennard-Jones, (2) Stock-Mayer and (3) Gay-Berne molecular interactions. This analysis is performed in terms of the miscibility parameter,  $\alpha = \epsilon_{AB}/\epsilon_{AA}$ , with  $\epsilon_{AA} = \epsilon_{BB}$ . When the miscibility of the mixture is in the range  $0 < \alpha < 1$ , a continuous critical line of consolute points appears. This line interscts the LV coexistence curve at different positions depending on the value of  $\alpha$ , yielding mainly three different topologies for the phase diagrams. We also carried out a detailed study of the interfacial properties as function of T and  $\alpha$ .

## Friday, March 17, 2006 8:00AM - 11:00AM -

Session Y8 DFD: General Fluid Dynamics Baltimore Convention Center 314

#### 8:00AM Y8.00001 DCOMP Award Lecture (Metropolis): A 3D Spectral Anelastic Hydrody-

namic Code for Shearing, Stratified Flows<sup>1</sup>, JOSEPH BARRANCO, Harvard University — We have developed a three-dimensional (3D) spectral hydrodynamic code to study vortex dynamics in rotating, shearing, stratified systems (eg. the atmosphere of gas giant planets, protoplanetary disks around newly forming protostars). The time-independent background state is stably stratified in the vertical direction and has a unidirectional linear shear flow aligned with one horizontal axis. Superposed on this background state is an unsteady, subsonic flow that is evolved with the Euler equations subject to the anelastic approximation to filter acoustic phenomena. A Fourier-Fourier basis in a set of quasi-Lagrangian coordinates that advect with the background shear is used for spectral expansions in the two horizontal directions. For the vertical direction, two different sets of basis functions have been implemented: (1) Chebyshev polynomials on a truncated, finite domain, and (2) rational Chebyshev functions on an infinite domain. Use of this latter set is equivalent to transforming the infinite domain to a finite one with a cotangent mapping, and using cosine and sine expansions in the mapped coordinate. The nonlinear advection terms are time integrated explicitly, whereas the Coriolis force, buoyancy terms, and pressure/enthalpy gradient are integrated semi- implicitly. We show that internal gravity waves can be damped by adding new terms to the Euler equations. The code exhibits excellent parallel performance with the Message mapping and protoplanetary disks and the Kelvin-Helmholtz instability in the dusty midplanes of protoplanetary disks.

 $^1 \mathrm{In}$  collaboration with Philip Marcus

8:36AM Y8.00002 Evaporating droplets , NOUSHINE SHAHIDZADEH-BONN, Laboratoire des Materiaux et Structures du Genie Civil (LMSGC), SALIMA RAFAI, WZI/University of Amsterdam, AZA AZOUNI, LMSGC, DANIEL BONN, LPS/Ecole Normale Superieure, LMSGC TEAM, LPS/ENS TEAM, WZI/UVA COLLABORATION — In our everyday life we are constantly confronted with evaporating drops and the consequences of it. The seemingly simple problem of an evaporating droplet has attracted a great deal of attention over the past years. The problem is complicated due to the fact that the form of the droplet during the evaporation is a priori unknown, and due to the large number of effects that have to be taken into account (temperature, convection, Marangoni effects...). We consider the very simple situation of the evaporation of a perfectly wetting liquid on a molecularly smooth surface. The radius R(t) of the droplet is followed in time until it reaches zero. If the evaporation is purely diffusive, a radius that decreases as the square root of time is lighter than air, and the vapor of other liquids more dense. If we carefully confine the water so that the difference is likely to be due to the fact that water vapor is lighter to the andri, if we force convection for an organic liquid, we retrieve the anomalous exponent for water.

8:48AM Y8.00003 Effect of Viscoelasticity on Drop Deformation , NISHITH AGGARWAL, University of Delaware, KAUSIK SARKAR, University of Delaware — Deformation of a drop is numerically investigated when one or both of the drop and continuous phases is viscoelastic. A three-dimensional front-tracking finite difference method is used to simulate the deforming drop. The viscoelasticity is modeled using the Giesekus and Oldroyd–B constitutive relations. In a shear flow, a viscoelastic drops in a Newtonian matrix deforms less than a Newtonian drop. Specifically, bounded viscoelastic drop shapes are found for capillary numbers where a Newtonian drop would break up. Matrix viscoelasticity, however is observed to cause non-monotonic change in drop deformation with increasing viscoelasticity. The effects of inertia, interfacial tension, viscosity ratio and imposed flow periodicity (in oscillatory shear) will be presented. The detailed results about transient dynamics, viscous and viscoelastic stresses and the velocity fields inside and outside the drop will be discussed and explained.

9:00AM Y8.00004 Pressure Driven Liquid-Vapor Phase Transitions, TIANSHI LU, ROMAN SAMULYAK, Computational Science Center, Brookhaven National Laboratory, JAMES GLIMM, Department of Applied Mathematics and Statistics, Stony Brook University — Liquid-vapor phase transitions driven by pressure waves have been studied analytically and numerically. The Stefan problem has been extended to incorporate the compressibility of the vapor phase. Both internal heat conduction and external heat deposition (such as from electrons in tokamak fusion reactors) have been considered. The steady state and the transient waves in the phase transitions have been investigated. A numerical scheme has been developed for the simulation of compressible two-phase flows with phase transitions in the frame of front tracking. Phase boundaries can be created dynamically in regions under critical conditions. The numerical method has been applied to the simulation of boiling and cavitating processes.

9:12AM Y8.00005 Interaction between a free boundary and thermal convection in an annulus , JIN-QIANG ZHONG, Physics Dept., NYU, JUN ZHANG, Physics Dept. and Courant Inst., NYU — We report an experimental study in turbulent thermal convection that has a free upper surface. The geometry of the convective system is annular with aspect ratio (girth/height) 6.8 and with periodic boundary condition. Our experiment studies the interaction between the convective flow and a freely moving floating boundary that partially covers the open surface. The floating boundary position and the corresponding convective pattern are recorded at the same time and are correlated to reveal the dynamics of the coupled system. Our experiment aims to illustrate the intricate mechanism of continental drift that is driven by mantle convection.

#### 9:24AM Y8.00006 The Stochastic Dynamics of an Array of Atomic Force Microscope Cantilevers in a Viscous Fluid, MATTHEW CLARK, Virginia Tech, MARK PAUL, Virginia Tech — The hydrodynamic coupling between micron scale atomic force microscope cantilevers in a viscous fluid is studied. Using the fluctuation-dissipation theorem, the stochastic dynamics of the cantilevers are quantified from deterministic calculations. Numerical simulations of individual cantilevers immersed in fluid are used to verify the approach. A simple harmonic oscillator model is shown to be reasonable for the description of the dynamics of a single cantilever. The fluid induced correlations in an array of cantilevers are then explored and quantified. Absolute predictions of the cross-correlations in the equilibrium fluctuations of cantilever displacement are presented. This is used to yield limits of the force and time scales of operation for a correlation method using multiple atomic force microscope cantilevers.

9:36AM Y8.00007 Co-rotating Batchelor vortex merging , PAULO FERREIRA DE SOUSA, New Mexico State University, JOSE CARLOS FERNANDES PEREIRA, Instituto Superior Tecnico — The dynamics of co-rotating vortex pairs without axial flow has been recently throughly studied through theoretical, experimental and numerical studies, which revealed different instabilities contributing to the decay of the vortices. In this paper the objective is to extend the analysis to the case of co-rotating vortices with axial flow at low Reynolds numbers. A high-order incompressible Navier-Stokes flow solver is used. The momentum equations are spatially discretized on a staggered mesh by finite differences and all derivatives are evaluated with 4th order compact finite difference schemes with RK-4 temporal discretization. The initial condition is a linear superposition of two co-rotating circular Batchelor vortices with q = 1. It is found that there is an initial evolution that resembles the evolution that single q = 1 vortices go through. Azimuthal disturbances grow and result in the appearance of large-scale helical sheets of vorticity. With the development of these instability waves, the axial velocity deficit is weakened. The redistribution of both angular and axial momentum between the core and the surroundings drives the vortex core to a more stable configuration, with a higher q value. After these processes, the evolution is somewhat similar to a pair of co-rotating Lamb-Oseen vortices. A three-dimensional instability develops, with a large band of unstable modes, with the most amplified mode corresponding scaling with the vortex initial separation distance.

9:48AM Y8.00008 Magnetic Body Force Sustained Temperature Gradient<sup>1</sup>, JONATHAN FRAINE, WEILI LUO, University of Central Florida, UNIVERSITY OF CENTRAL FLORIDA TEAM — The temperature gradient was established in a magnetic fluid by controlling the rate of cycling coolant. Measurements were done to monitor temperature gradient verses time before and after the cooling was stopped in both zero and applied magnetic field. We found that the magnetic field can sustain a larger temperature gradient. The theoretical calculation shows that the effect of field on the temperature gradient is attributed to the magnetic body force that depends on the gradient of the susceptibility.

<sup>1</sup>This work is partially supported by NSF NIRT 0103587.

10:00AM Y8.00009 Shock Interaction with a Finite Thickness Two-Gas Interface , JOHN LABENSKI, NIST, YONG KIM, Lehigh University — A dual-driver shock tube was used to investigate the growth rate of a finite thickness two-gas interface after shock forcing. One driver was used to create an argon-refrigerant interface as the contact surface behind a weak shock wave. The other driver, at the opposite end of the driven section, generates a stronger shock of Mach 1.1 to 1.3 to force the interface back in front of the detector station. Two schlieren systems record the density fluctuations while light scattering detectors record the density of the refrigerant as a function of position over the interface during both it's initial passage and return. A pair of digital cameras take stereo images of the interface, as mapped out by the tracer particles under illumination by a Q-switched ruby laser. The amount of time that the interface is allowed to travel up the driven section determines the interface and its growth due to shock forcing. The results show that the interface has a distribution of thicknesses and that the interaction with a shock further broadens the interface.

10:12AM Y8.00010 Investigation of Oxygen Transfer Enhancement in Thermally Driven Cavities By Lattice Boltzmann Simulation., HUIDAN YU, CNLS, Los Alamos National Lab, JINSUO ZHANG, D-5, Los Alamos National Lab, NING LI, MST-10, Los Alamos National Lab — We investigate the enhancement of mass transfer in 2D thermally driven cavities using lattice Boltzmann equation (LBE) method. The computational technique integrates three coupled LBEs for solving velocity, temperature, and concentration fields simultaneously. Simulation is performed for oxygen transfer in lead/lead-bismuth eutectic with variations of temperature boundary, Schmidt number, and field aspect ratio to investigate the effects on enhancement of oxygen transfer. Interested characteristics include oxygen concentration, Sherwood number, and velocity profiles, etc. Our results clearly indicate that oxygen transfer is dominated by convection while diffusion also plays a role on it. Comparative studies demonstrate that side heating and top cooling device is more efficient to transfer oxygen than side heating and cooling device and oxygen transfers more rapidly in square cavity than in rectangular cavity. This work establishes a reliable thermal LBE model for thermally driven heat and mass transfer.

10:24AM Y8.00011 Energy from Ocean Waves, River Currents, and Wind, SHYAMAL GUHA, Texas Southern University — The Earth we live in is surrounded by fluids, which are in perpetual motion. The air in the atmosphere and water found in lakes, ocean, and rivers form our natural environment. Much of the fluid medium is in constant motion. The kinetic energy of this moving fluid is astronomical in magnitude. Over the years, I have considered methods of converting a fraction of the vast reserve of this kinetic energy into electro-mechanical energy. I have conceived a few schemes of such conversions. The fluids whose kinetic energy can be converted into electro-mechanical energy are the following: ocean waters, river currents and atmospheric air. In a book to be published in the spring of 2006, I have described different techniques of energy conversion. In the upcoming APS meeting, I plan to discuss some of these techniques.

10:36AM Y8.00012 Motion of Rigid Bodies in Newtonian and non-Newtonian Fluids , ASHWIN VAIDYA, Florida State University — The properties of non-Newtonian fluids, such as normal stress effects and non-constant viscosities are known to result in flow phenomenon which are dramatically different from those of Newtonian fluids. One such interesting difference in the behavior of these kinds of fluids is in their interaction with submerged rigid bodies. In this talk, we will focus on the problem of steady motions of symmetric rigid bodies as they freefall in Newtonian and viscoelastic fluids, modeled by the Navier Stokes, Power Law, Second order and the Generalized Second order fluid models. We will examine how variations in forces and torques in these two kinds of fluids can result in remarkably different phenomenon.

10:48AM Y8.00013 Particle Dynamics in Low Reynolds Number Fluidized Beds, PHIL SEGRE, Physics Dep., Emory Univ., Atlanta Ga., JIM MCCLYMER, Physics Dep., Univ. of Maine, Orono ME — The sedimentation dynamics of extremely low polydispersity,  $\sigma_a/a \sim 1.5\%$ , non-Brownian, particles are studied in a liquid fluidized bed at low Reynolds number,  $Re \ll 1$ . When fluidized, the system reaches a steady state in which the local velocity fluctuations and particle concentration are found to become highly stratified with height in the column. Results are presented for the degree of stratification with normalized bed height H/a. We find that taller beds are more stratified than shorter beds. However, recent computer simulations have not found any measurable stratification with height. We reconcile this apparent disagreement by showing that the stratification in experiments of comparably small systems such as those studied by simulation are indeed very small. We also develop a simple advection-diffusion model that connects the velocity fluctuations to the concentration gradients, and account for the observed bed stability.