Monday, March 16, 2009 8:00AM - 10:48AM –
Session A14 DFD: Instabilities, Turbulence and Nonlinear Flows 315

8:00AM A14.00001 Search for the “ultimate state” in turbulent Rayleigh-Bénard convection for Rayleigh numbers up to $4 \times 10^{13}$ and Prandtl numbers near 0.8.1 GÜNTHER AHLERS, UCSB, DENIS FNSCHILLING, CNRS NanCey, EBERHARD BODENSCHATZ, MPI for Dyn. and Self-org., Goettingen — Measurements of the Nusselt number $Nu$ over the Rayleigh-number range $10^{10} < Ra < 4 \times 10^{13}$ for $N_2$ (Prandtl number $Pr = 0.72$) and $SF_6$ ($Pr = 0.78$ to 0.82) are reported. They were made at pressures up to 15 bars and near-ambient temperatures for a cylindrical sample of height $L = 2.2 \text{ m}$ and diameter $D = 1.1 \text{ m}$ in a new High-Pressure Convection Facility (HPCF) constructed at the Max Planck Institute for Dynamics and Self-Organization in Göttingen, Germany. The data can be represented well by a power law with an effective exponent of 0.31. They do not show the transition to an “ultimate regime” reported by Chavanee et al.

1Work at UCSB supported by NSF Grant DMR07-02111.

8:12AM A14.00002 Large-scale circulation and Nusselt number in turbulent rotating Rayleigh-Bénard convection.1 JIN-QIANG ZHONG, UCSB, RICHARD STEVENS, U. Twente, HERMAN CLERCX, Eindhoven U. Tech., DETLEF LOHSE, U. Twente, GÜNTHER AHLERS, UCSB — We present measurements of the large-scale circulation (LSC) and the Nusselt number $Nu$ of turbulent Rayleigh-Bénard convection in a cylindrical cell of aspect ratio 1 and rotated about a vertical axis at a rate $\Omega$. The side-wall temperatures at eight equally spaced azimuthal positions in the horizontal mid-plane were fit to a cosine function that gave the azimuthal LSC orientation $\theta(t)$ (1 is the time), the temperature amplitude $\delta(t)$, and the rms amplitude $\delta_{\text{rms}}(t)$ of the fluctuations about the fits. The LSC precessed in an azimuthal direction opposite to that of the imposed rotation. The precession rate $\omega = d\theta/dt$ showed a sharp transition at a Rossby number $Ro^* \approx 2.5$. As $\Omega$ increased, $d\theta/dt$ increased and $\delta_{\text{rms}}(t)$ increased beginning at $Ro^*$. At $Ro^* \approx 6$, $Nu$ began to increase with increasing $\Omega$. At high $\Omega$, $|\omega|$ was proportional to but much smaller than $\Omega$.

1Work at UCSB supported by NSF Grant DMR07-02111.

8:24AM A14.00003 Geometry of turbulence: a stroll through 61,506 dimensions1. PREDRAG CVITANOVIC, JOHN F. GIBSON, Georgia Tech, JONATHAN HALCROW, Inst. for Physical Sciences, McLean, VA 22101 — We propose to use a hierarchy of $\omega$-amplitude azimuthal positions in the horizontal mid-plane were fit to a cosine function that gave the azimuthal LSC orientation $\theta(t)$ (1 is the time), the temperature amplitude $\delta(t)$, and the rms amplitude $\delta_{\text{rms}}(t)$ of the fluctuations about the fits. The LSC precessed in an azimuthal direction opposite to that of the imposed rotation. The precession rate $\omega = d\theta/dt$ showed a sharp transition at a Rossby number $Ro^* \approx 2.5$. As $\Omega$ increased, $d\theta/dt$ increased and $\delta_{\text{rms}}(t)$ increased beginning at $Ro^*$. At $Ro^* \approx 6$, $Nu$ began to increase with increasing $\Omega$. At high $\Omega$, $|\omega|$ was proportional to but much smaller than $\Omega$.

1Partly supported by NSF grant DMS-0807574

8:36AM A14.00004 Lagrangian and Eulerian Turbulence: intermittency and Universality. LUCA BIFERALE, University of Rome, ICTR COLLABORATION — We present the result of a high resolution numerical simulations of homogeneous and isotropic turbulence at $Re \sim 600$. We discuss a phenomenological bridge-relation able to capture intermittent fluctuations in inertial and viscous scales for both Eulerian and Lagrangian ensembles.

8:48AM A14.00005 Large-eddy simulation of swirling reacting flows. MARCEL ILIE, University of California San Diego — Turbulent, swirling flows are encountered frequently in various chemical engineering processes. In combustion processes swirling flames are of interest due to the fact that provide enhanced mixing and reduce the pollutants formation. The challenge in understanding turbulent swirling flows stems mainly from the complexity of the flow field which is subject to vortex breakdown, recirculation and flow instability. In general the flow instabilities arise at high swirl numbers and can be used to control the performance of combustors. In the present study a large-eddy simulation (LES) approach with Smagorinsky eddy viscosity subgrid scale model is used to predict the swirling flame. The conserved scalar mixture fraction-based thermo-chemical variables are described using the steady laminar flamelet model. The present study shows that LES together with a laminar flamelet model provides a good prediction of the structure of turbulent swirling flames. Also LES captured very well the complex flame structures involving vortex breakdown which leads to swirl-induced recirculation zones, flow instability, and the occurrence of localized extinction. Also, the present study shows that the formation of an elongated recirculation (bluff-body stabilized) zone is strongly dependent on the swirl number and the ratio of momentum in the swirling annulus and central fuel jet.

9:00AM A14.00006 Methods to Approach Velocity Data Reduction and Their Effects on Conformation Statistics in Viscoelastic Turbulent Channel Flows. GAURAB SAMANTA, ANTONY BERIS, University of Delaware, ROBERT HANDLER, Naval Research Laboratory, KOSTAS HOUSIADAS, Aégean University, Greece — Karhunen-Loève (KL) analysis of DNS data of viscoelastic turbulent channel flows helps us to reveal more information on the time-dependent dynamics of viscoelastic modification of turbulence [Samanta et. al., J. Turbulence (in press), 2008]. A selected set of KL modes can be used for a data reduction modeling of these flows. However, it is pertinent that verification be done against established DNS results. For this purpose, we did comparisons of velocity and conformation statistics and probability density functions (PDFs) of relevant quantities obtained from DNS and reconstructed fields using selected KL modes and time-dependent coefficients. While the velocity statistics show good agreement between results from DNS and KL reconstructions even with just hundreds of KL modes, tens of thousands of KL modes are required to adequately capture the trace of polymer conformation resulting from DNS. New modifications to KL method have therefore been attempted to account for the differences in conformation statistics. The applicability and impact of these new modified KL methods will be discussed in the perspective of data reduction modeling.

9:12AM A14.00007 Study of Influence of Rapid Pressure in MHD Turbulence. SAIKISHAN SURAYANAYAN, AARTHI SEKARAN, Texas A&M University — Turbulence, under the influence of magnetic field is characterized by anisotropy. Relatively limited work has been done in understanding and modeling magnetohydrodynamic (MHD) turbulence.The rapid distortion theory (RDT), which has been employed to study hydrodynamic turbulence, is a limiting case where the gradients of the mean velocity are very high compared to the gradients of the fluctuating field. When analyzed in a spectral framework, this leads to the independent evolution of each Fourier mode. RDT has been used to understand production and more importantly the “rapid” part of the pressure strain redistribution, as the other terms in the Reynolds stress evolution equation become negligible in the rapid distortion limit. Earlier work attempts to characterize the effect of the rapid pressure based on the geometry of the symmetric part of the mean velocity gradient tensor. This work deals with the application of RDT to MHD turbulence. The application of Elsasser variables reorganizes the MHD equations in a form similar to conventional Navier-Stokes. The current work is a numerical study of the Elsasser variable evolution equation in the rapid distortion limit and attempts to understand the role of the rapid magnetic pressure in the evolution of the Reynolds stresses for different mean distortions and magnetic fields.
9:24 AM A14.00008 Anisotropic Particles in Fluid Flow1, MONICA KISHORE, Haverford College, NICHOLAS T. OUELLETTE, Yale University, JERRY GOLLUB, Haverford College — Anisotropic particles are common in natural flows. In previous work [1] the dynamics of neutrally buoyant finite-sized spherical particles with Stokes numbers up to 0.08 were examined in 2D flows with Reynolds numbers of 72-220. Here, we extend this work to neutrally buoyant, high-aspect-ratio anisotropic particles of mm to cm length in a 2D cellular flow. The particle trajectories and orientations are tracked simultaneously with the underlying velocity field, which is measured using much smaller tracer particles. These methods allow us to compare the relative velocity and orientation of anisotropic particles to various features of the flow field. We find, for example, that the long axes of the particles preferentially align with the instantaneous direction of maximum compression, and that this alignment increases with particle aspect ratio. [1] N.T. Ouellette, P.J.J. O'Malley, and J.P. Gollub, Phys. Rev. Lett. 174504 (2008).

1Supported by NSF-DMR 0803153.

9:36 AM A14.00009 Statistics of preferential particle concentration in free-surface1, JASON LARKIN, WALTER GOLDBURG, University of Pittsburgh, MAHESH BANDI, Center for Nonlinear Studies and Condensed Matter & Thermal Physics Group, Los Alamos National Laboratory — Particles floating on a turbulent surface of water cluster into temporally complex patterns. We experimentally study the statistics of this preferential particle concentration for various Reynolds numbers, for both transient and steady-state dynamics. The probability density function for particle concentration exhibits a power-law with an exponential cut-off. We will discuss our preliminary analysis as to how this distribution depends upon the Reynolds number and the spatial-scale r at which the system is coarse-grained.

1This work supported by National Science Foundation grant DMR NSF 0604477. MMB carried out this work under the auspices of the National Nuclear Security Administration of U.S. Department of Energy at LANL under contract No. DE-AC52-06NA25396.

9:48 AM A14.00010 Vortex Street behind an Oscillating Wire on a Soap Film, AARON MEYER, ILDOO KIM, X.L. WU, University of Pittsburgh — A von Kármán vortex street, a periodic array of vortices behind a bluff body is normally characterized by a single frequency $f_0$ at which the vortices shed. In this study, von Kármán vortex streets are generated on a 2D soap film using a glass-covered metal wire in a static magnetic field. When the wire is driven with electric current to make an oscillatory motion with frequency $f_e$, transverse to the mean flow, vortices shed at a frequency $f'$ differs from $f_0$. It is seen that with oscillation, $f_0$ is suppressed. $f'/f_0$ becomes a rational number, and vortices are rearranged to form an exotic spatial structure. This "frequency-locking" phenomena show some features of the sine-circle map, but the relevancy to the physical system is not clear. When the amplitude of the oscillation is large enough, the system becomes chaotic. In this chaotic regime, the energy power spectrum resembles that of 2D decaying turbulence.

10:00 AM A14.00011 An Anomalous Behavior in Vortex Shedding in a Flowing Soap Film, ILDOO KIM, X.L. WU, University of Pittsburgh — It is generally believed that von Kármán vortex street is characterized only by Reynolds number $Re = UD/\nu$, where $U$ is the mean flow speed, $D$ is the size of the body which generates the vortex street, and $\nu$ is the kinematic viscosity. In this study, we present experimental data in a flowing soap film showing that changing $U$ with fixed $D$ and changing $D$ with fixed $U$ are not equivalent to each other, suggesting that $Re$ alone is not sufficient to characterize vortex shedding by a bluff body. The velocity of eyes of the vortices relative to the mean flow, normalized by $U$, increases when we increase $D$, but decreases when we increase $U$. It is also found that the longitudinal spacing between the eyes is a linear function of $D$, but independent of $U$.

10:12 AM A14.00012 Rayleigh-Taylor Instability in Nonlinear Optics, SHU JIA, JASON W. FLEISCHER, Princeton University — We demonstrate, theoretically and experimentally, an all-optical Rayleigh-Taylor instability. By applying a polar (Madelung) transformation to the nonlinear Schrödinger equation for paraxial beams, we identify fluid density with light intensity and fluid velocity with the gradient of the optical phase. Pressure is obtained by using a self-defocusing nonlinearity in a photorefractive crystal, while acceleration is created by imposing a refractive index gradient. In this way, we are able to control the effective gravity, pressure, and input density ratio. The perturbed interface at the output is then studied as a function of these parameters. Observations of the characteristic spatial period show excellent agreement with analytical calculations from perturbation theory. In this case, wave diffraction, rather than viscosity or surface tension, sets the scale for long-wave growth. Further, we show that compressibility effects are important and demonstrate that care must be taken regarding shock-wave formation. The results hold for any Schrödinger fluid, e.g. superfluids and quantum plasma, and lay the foundation for a variety of fluid-inspired instabilities in nonlinear optics.

10:24 AM A14.00013 Dispersive shock waves with negative pressure, WENJIE WAN, DIMITRI DYLOV, CHRISTOPHER BARSIL, JASON FLEISCHER, Princeton University — Dispersive shock waves (DSWs) arise from nonlinear wave breaking and mode dispersion and are a fundamental type of fluid behavior. In normal fluid systems, the pressure is positive and repulsive, so that the underlying particles resist compression. Examples include water, plasma, and optical beams with self-defocusing nonlinearity. However, there are systems in which the interactions are attractive, resulting in an effectively negative pressure. Here, we demonstrate that dispersive shock waves can arise in these negative-pressure systems by considering the equivalent optical problem with self-focusing nonlinearity. Using partially-coherent light, to prevent the competition of modulation instability, we experimentally observe DSWs formed in a self-compressive beam in a photorefractive crystal. We characterize the nonlinear speed and profile of the DSWs and show that statistical de-phasing by the incoherent beam causes an effective Landau damping of the waves. Observations are supported both by analytic theory and numerical simulation.

10:36 AM A14.00014 Convective instability in pipe flow through a sudden expansion, JAMES SEDDON, University of Manchester — Flow through a sudden expansion in a pipe has been the subject of a lot of recent scientific interest. The geometry occurs in many industrial processes, from heat exchangers to combustion chambers, and is closely related to the physiological problem of flow through a stenosis. The inlet flow from the upstream pipe is Poiseuille, which forms a central jet surrounded by a recirculating eddy in the expanded downstream pipe. Recently we showed that this kind of flow passes through a symmetry breaking bifurcation before the onset of both intermittent and fully periodic time-dependent effects. We have now investigated the intermittency in more detail and find that the flow becomes convectively unstable. A wave packet emerges from the laminar state and grows to a maximum size of several diameters before decaying.
8:00AM A15.00001 Impact of a viscous drop, WENDY W. ZHANG, ROBERT D. SCHRÖLL, University of Chicago, CHRISTOPHE JOSSENDRE, STEPHANE ZALESKI, UMR 7190, Institut d’Alembert — Recent experiments [1] reveal that reducing the ambient air pressure entirely suppresses the splash generated by the impact of an oil drop at several m/s onto a dry smooth wall. Motivated by these observations, we simulate two types of drop impact: impact onto a smooth, dry solid wall and head-on collision of two identical liquid drops. In both cases we make the additional simplification that impact simply arrests the downward fall and redirects the liquid radially outwards in a thin, expanding sheet. It does not break the drop surface. Since experiments suggest that splash is created by airflow deforming the thin sheet, we focus on the time-evolution of the thin liquid sheet but restrict ourselves to a simpler situation of negligible airflow effects. In this regime, we find that the ejected sheet is always characterized by two different length-scales. Surface tension controls the rim size. The thickness over the rest of the sheet is controlled by a different mechanism. Impact onto a solid surface creates a pancake whose thickness is controlled by viscous dissipation. Head-on collision creates a sheet that thins continuously with distance from the collision center. Its thickness is controlled by the kinematics of impact.


8:12AM A15.00002 Focused impact through layers of aqueous cornstarch solution, BIN LIU, Courant Institute, NYU, JUN ZHANG, Dept. of Physics and Courant Institute, NYU, MICHAEL SHELLEY, Courant Institute, NYU — A layer of aqueous cornstarch solution, when punched with a solid sphere, will create a thickened mass on the sphere that transmits the impact towards the bottom. As a consequence, the mass can leave an imprint on the bottom, if composed of a soft molding clay. The impact transmitted through the fluid layer is more localized for slower speeds of the sphere, giving rise to an imprint with sharper curvature. Our work shows that a layer of shear-thickening fluid may help to focus the impact rather than dissipate it when punched slowly enough.

8:24AM A15.00003 Drop pinch-off of concentrated surfactant solutions in the lamellar phase, ITAI COHEN, Cornell University, PATRICK SPICER, MARCO CAGGIONI, P&G, JOHN SAVAGE, Cornell University — Droplet pinch-off in air is a common phenomenon that occurs all around us. At the point of pinch-off, the drop radius shrinks to zero in a finite amount of time. The pressure exerted by the interface is such that it forms a flat rim of minimal thickness. It becomes singular at Pinch-off. In Newtonian fluids, this finite time singularity gives rise to universal features in the pinch-off process that can be described by similarity solutions for the fluid air interface. In this talk I will address the question of how this process is altered when observed in concentrated surfactant solutions that are in the lamellar phase. Remarkably we find that pinch-off in these systems is a mix between universal and non-universal behavior.

8:36AM A15.00004 Watching the Paint Dry: Dynamics of Drying in Porous Media, LEI XU, Harvard University, SIMON DAVIES, ICI, ANDREW SCHMIDT, the University of Edinburgh, DAVID WEITZ, Harvard University — What is the dynamics of drying in porous media? It has been difficult to visualize due to the non-transparency of the media. We study this phenomenon in an optical index matched colloidal system with confocal microscopy. We observe abrupt air invasions which result from the strong flow from menisci in large pores to menisci in small pores. The size and structure of the air invasions are in accord with 3D invasion percolation. By varying the particle size and contact angle we unambiguously demonstrate that capillary pressure dominates the drying process.

8:48AM A15.00005 Monitoring Three-dimensional Fluid Configurations in Porous Media, AMBER KRUMMEL, DAVID WEITZ, Harvard University, SCHLUMBERGER COLLABORATION — The spatial and time resolution of confocal microscopy affords us the ability to study three-dimensional dynamics. We observe capillary drying of a sample. The drying process is studied with a confocal microscope with precise flow measurements, such that we can begin to understand the origins and consequences of the three-dimensional fluid configurations that evolve in the sample. The porous media used in this work is composed of slightly sintered, borosilicate glass beads that are 150 microns in diameter.

We appreciate generous support from Schlumberger.

9:00AM A15.00006 Shear banding fluids in microchannels: high shear rheology, slippage and Poiseuille flow instability, PHILIPPE NGHE, GUILLAUME DEGRE, PATRICK TABELING, MMN, UMR CNRS-ESPCI 7083 Gulliver, ARMAND AJDARI, PCT, UMR CNRS-ESPCI 7083 Gulliver — We characterize by Particle Image Velocimetry the Poiseuille flow a semi-dilute solution of wormlike micelles (a CTAB and sodium nitrate aqueous solution) in pressure resistant microchannels. At low shear rates, we observe a parabolic profile. Increasing the pressure driving the flow, the fluid separates into two phases above a critical shear rate at the wall. This is the so called shear-banding regime. Deducing the non-linear rheology from the velocity profiles by a local calculation, we are able to measure the stress versus shear rate curve at least one order of magnitude above the dynamical range attainable in Couette geometries, independently from the slippage, revealing a strongly shear-thinning structure. In addition, by extrapolation of the velocity profiles to the wall position, we measure an absence of slippage at the wall. Looking into more details to the increase in velocity fluctuations in the downstream direction, we characterize a supercritical instability in this shear-banded Poiseuille flow, localized at the interface between the two phases with a wavelength comparable to the confining dimension.

9:12AM A15.00007 Nonlinear Dynamics in Viscoelastic Jets, TRUSHANT MAJMUDAR, MATTTHIE VARAGNAT, GARETH MCKINLEY, Massachusetts Institute of Technology — Instabilities in free surface continuous jets of non-Newtonian fluids, although relevant for many industrial processes, remain poorly understood in terms of fundamental fluid dynamics. Inviscid, and viscous Newtonian jets have been studied in considerable detail, both theoretically and experimentally. Instability in viscous jets leads to regular periodic coiling of the jet, which exhibits a non-trivial frequency dependence with the height of the fall. Here we present a systematic study of the effect of viscoelasticity on the dynamics of continuous jets of worm-like micellar surfactant solutions of varying viscosities and elasticities. We observe complex nonlinear spatio-temporal dynamics of the jet, and uncover a transition from periodic to quasi-periodic to a multi-frequency, broadband-spectrum dynamics. Beyond this regime, the jet dynamics smoothly crosses over to exhibit the “leaping shampoo” or the Kaye effect. We examine different dynamical regimes in terms of scaling variables, which depend on the geometry (dimensionless height), kinematics (dimensionless flow number), and the fluid properties (elasto-gravity number) and present a regime map of the dynamics of the jet in terms of these dimensionless variables.

9:24AM A15.00008 Relating shear banding and orientational order in wormlike micellar solutions, MATTHEW HELGESON, MATTHEW REICHERT, University of Delaware, ERIC KALER, Stony Brook University, NORMAN WAGNER, University of Delaware — Shear banding has been observed in a variety of complex fluids, including polymer solutions, colloidal suspensions and, most prominently, wormlike micelles (WLMs). However, accurate modeling of shear banding fluids remains a challenge, due to the inability to identify the mechanism(s) leading to banding. Using a novel approach that combines measurements of phase behavior, rheology, and spatially-resolved microstructure on model WLMs, we present the first complete study of local rheology and microstructure through the shear banding transition for model WLMs in the vicinity of an equilibrium isotropic-nematic transition (I-N). The rheology of such fluids is well-described by the Giesekus constitutive equation with incorporated stress diffusion, which allows simultaneous description of rheology, flow kinematics, and spatially-resolved microstructure under shear. The results show that shear banding coincides with a first-order, shear-induced transition to a paramesomorphic state at critical values of micellar orientation and alignment, which can be related directly to a non-monotonic constitutive relation. Furthermore, the model allows for the construction of non-equilibrium state diagrams that elucidate a number of experimental observations in shear banding fluids.
9:36AM A15.00009 Structure and Phase Behavior of Ion–Dipole Mixtures. WONKI ROH, ERIK LUIJTEN, University of Illinois at Urbana-Champaign — It is well established that Coulombic interactions induce a liquid–liquid transition in ionic solutions. By contrast, the occurrence of phase separation driven by anisotropic dipolar interactions is still a matter of debate, with our recent simulation results excluding this phase separation for a large region of the temperature–density plane. These observations naturally lead to the question whether phase separation takes place in mixtures that contain ionic species in addition to dipolar polar species. Employing large-scale grand-canonical Monte Carlo simulations, we investigate four prototypical ion–dipole mixtures: ion-dominated systems in which the dipole moment is either strong or weak, and dipole-dominated systems with strong or weak dipolar character. We focus on the low-temperature regime and search for phase separation by varying the chemical potentials of the ions as well as the dipolar particles. Depending on temperature and on the magnitude of the dipole moment, remarkable liquid structures are found that may have implications not only for the behavior of ion–dipole mixtures, but also for self-assembly in suspensions containing charged and dipolar colloids.

9:48AM A15.00010 Surface Layering Near Room Temperature in a Nonmetallic Liquid. SUDESHNA CHATTOPADHYAY, BENJAMIN STRIPE, PHILIP SHIVELY, GEUNNADI EVMENENKO, PULAK DUTTA, Dep. of Physics & Astronomy, Northwestern Univ., STEVEN EHRlich, HAIDING MO, Brookhaven National Laboratory — Oscillatory density profiles (layers) have been observed at the free surface of an organic liquid metal and above room temperature. A surface-layered state has been previously reported only in one dielectric liquid, tetraethylsilane (TEOS), and only at lower temperatures [2]. We have used x-ray reflectivity to study a molecular liquid, pentaphenyl trimethyltrisiloxane. Below T = 267K (well above the freezing point for this liquid), density oscillations appear at the surface. This liquid has a higher Tc (2000K) than TEOS (590K), so that layers appear at T/Tc = 0.2 in both cases. Our results indicate that surface order is a universal phenomenon in both metallic and dielectric liquids, and that the underlying physics is likely to be the same since layers always appear at T < 0.2Tc as theoretically predicted [3].

REFERENCES:

1Supported by NSF grant no. DMR-0705137.

10:00AM A15.00011 Structural effect of sugars on water. SIMCHA SREBNiK, RAViT MATZA, ILYiA KUSNER, YOVAV D. LIVNEY, Technion - Israel Institute of Technology — The modulation of the structure of liquid water by solutes has tremendous consequences in numerous fields, particularly on the stability of proteins. However, the reasons for the differences in effects of similar solutes are still unclear. Recently, Livney and coworkers [1] found a strong relationship between the hydration layer of sugars and its effect on the phase transition of a model polymer, which may be explained by the strong interaction between water and sugars leading either to cooperative structuring of the water and thus to large hydration numbers, or disrupting water structure near the sugar, resulting in lower hydration. Using atomic Monte Carlo simulation, we studied the compatibility of various sugars with an ideal tetrahedral water structure, as embodied in hexagonal ice. Our simulations suggest the following order of compatibility with ideal water structure: galactose > glucose > mannose. In agreement, experimental measurements of isentropic compressibility show the same order of hydration numbers and structural effect. A simple physical model of the binary system is used to shed further insight on the structuring effect of sugars on water. 1. Shipgelman, A.; Portnaya, I.; Ramon, O.; Livney, Y. D. J Polym Sci Part B: Polym Phys 2006, 46, 2307-2318.

1Israel Science Foundation is acknowledged for partial support.

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10:12AM A15.00012 Reconstructing the dynamical solvent structure around a model ‘hydrated electron’ using inelastic x-ray scattering. R. CORDIAN, G.H. LAI, N. SCHMIDT, Dept of Physics, P. ABBAMONTE, Dept of Physics, Seitz Materials Research Lab, G.C.L. WONG, Depts of Mat. Science, Eng. and Physics, and Seitz Materials Research Lab, U of Illinois, Urbana-Champaign, R. CODEWAT, S. GARDE, Dept of Chem and Bio Engineering, Rensselaer Polytechnic Institute, M. KRISCH, European Synchrotron Radiation Facility, A.Q.R. BARON, SPriNG8/RIKEN and SPriNG8/JASRI — The structure and dynamics of water on femtosecond timescales is relevant to many topics in physical electronics using inelastic x-ray scattering. The imaginary part of density propagator \( \langle q, \omega \rangle \) is directly extracted from the IXS data, and the real part recovered using Kramer–Kronig relations. The result is complex-valued \( \chi(q,\omega) \) is the Fourier transform of the real-space density–density response function \( \chi(r,t) \) which measures the dynamical density fluctuations of water due to a point-like instantaneous impulse. We use this density propagator and linear-response theory to reconstruct a model of the hydrated electron. The water density fluctuations as the electron ‘diffuses’ through bulk water can be observed. Moreover, preliminary data on the solvent response to changes in the electronic wave function will be presented.

10:24AM A15.00013 Direct measurement of negative square gradient coefficients for density fluctuations in all-atom simulations of common liquids. COLIN DENNISTON, LINGTI KONG, DAN VRIESINGA, University of Western Ontario — We perform all-atom simulations of common liquids such as water (TIP3P) and organic liquids such as short-chain olefins. We show that square gradient coefficients for the mass density can be measured directly in a linear response measurement to sinusoidal forces at several different wavelengths. Surprisingly, in all fluids measured, the square gradient coefficient is negative implying that density gradients lower the free energy of the system. However, stability is maintained at any wavelength greater than the separation between molecules due to the global mass conservation constraint. We suggest that this provides a mechanism for the molecular scale cut-off of pressure singularities that arise in situations such as droplet pinch-off.

10:36AM A15.00014 Chiral Structures of Thermoresponsive Soft Spheres in Hollow Cylinders. MATTHEW A. LOHR, University of Pennsylvania, AHMED ALSAYED, CNRS/University of Pennsylvania, ZEKIN ZHANG, ARJUN G, YODH, University of Pennsylvania — We experimentally observe the formation of closely packed crystalline structures in hollow cylinders. The structures have varying degrees of chiral order. The systems are created from aqueous suspensions of thermoresponsive N-isopropylacrylamide (NIPA) microgel particles packed in micron-diameter glass capillaries. We categorize these structures according to classifications used by Erickson for tubular packings of hard spheres [1]. By varying the temperature-tunable diameter of these particles, the system’s volume fraction is changed, permitting observations of the resilience of these structures and their melting transitions. Melting of these structures is observed. [1] R. O. Erickson, Science 181 (1973) 705-716.

2This work is supported by MRSEC grant DMR-0520020 and NSF grant DMR-080488.

10:48AM A15.00015 Nonlinear Transverse Wave Excitations in Fluid Flows. DILLON SCOFIELD, Dept. Physics, Oklahoma State Univ., PABLO HUQ, Univ. Delaware — The interplay of inertia and dissipation in flows with nonlinear transverse wave excitations is described by including a vortex field into the stress-energy balance equation. The theory uses an acoustic spacetime which allows limiting the speed of propagation of fluid transverse waves to a maximum speed. In the low speed limit, the theory reduces to the Navier-Stokes equations. Comparison of the theory to experiment, relative to the Navier-Stokes theory, shows that the presence of the vortex field accounts for the observed relative increase in energy dissipation, extended lifetime of vortex structures, and excitation structure of the transverse wave field.
11:51 AM B14.0002 Experimental Study of Brownian Dynamics of Bent-core Colloidal Particles

12:03 PM B14.0003 Pinch-Off Dynamics of Non-Newtonian Fluids

12:15 PM B14.0004 Melting Dynamics of 3D Hard Sphere Colloidal Crystals

12:27 PM B14.0005 Multiple-Stage Melting and Freezing of Colloidal Crystallites with Short-range Attraction

12:39 PM B14.0006 Melting and Freezing of Colloidal Crystals on Strained Substrates

12:51 PM B14.0007 Transport and Sedimentation of Suspended Particles in Fracture Channels
Middle Tennessee State University.

viscosities of a newborn and unborn bovine serum with a different concentration of antibodies.

work, we have demonstrated that OT can be used to precisely measure the viscosity of biological fluids. Using an infrared laser trap directly proportional to the viscosity of the fluids. Therefore, calibration of the trap depends on the viscosity of the fluid which depends on temperature. In this properties of microscopic living biological systems like red blood cells. These studies are based on measurement of deformations caused by a force exerted

ANTHONY FARONE, MARY FARONE, Middle Tennessee State University — An optical tweezer (OT) has been widely used to study the mechanical

cavitation, typically occurring near the bottom edge. We make numerical estimates of the relevant physical parameters, and compare these with experimental

Hitting the top of a beer bottle, nearly full of water, with an open hand can cause the bottle to break, with the bottom separating from upper section. We

FONTANA, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University, MICHAEL SHELLEY, Courant Institute, New York University —

RAIN results in wet shoes, and often, wet feet. We describe a peculiar transport process associated with walking on wet surfaces which results in the vamps, and

GRIER, New York University — State Diagram for Optical Tweezers Induced Brownian Motors Bo Sun and David G. Grier Center for Soft Matter Research

localization length scale changes with the area fraction of the colloids. Dragged particle, as well as the perturbed motion of the surrounding particles. These responses are localized around the dragged particle, and we study how the localization length scale changes with the area fraction of the colloids.

ZACH NADLER, CARA HAGEMAN, VIKRAM PRASAD, ERIC R. WEEKS, Physics Dept., Emory University — We study polystyrene colloids placed at an oil-water interface as a quasi-two-dimensional colloidal system. As the area fraction of the colloidal particles is increased, we see liquid, hexatic, and crystalline phases. The liquid phase is structurally disordered; the hexatic phase has long range orientational order but poor translational order, and the crystalline phase has long range orientational and translational order. We classify these different phases using structural and dynamic parameters from prior work. Using a laser tweezer we trap and drag a particle along the interface and observe its effect on the surrounding colloids. Our interest is in how the response changes near phase transition boundaries, where the ordering of particles can qualitatively change. We characterize the response by the structural defects induced by the dragged particle, as well as the perturbed motion of the surrounding particles. These responses are localized around the dragged particle, and we study how the localization length scale changes with the area fraction of the colloids.

11:15AM B15.00001 Walking on water: why your feet get wet, MICHAEL SHELLEY, Courant Institute, New York University, JAKE FONTANA, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University — Walking on wet pavement during or after heavy rain results in wet shoes, and often, wet feet. We describe a peculiar transport process associated with walking on wet surfaces which results in the vamps, and frequently, the insides, of shoes getting wet. We discuss details of this process and compare experimental results with simple model predictions. Strategies for keeping feet dry will be considered.

11:27AM B15.00002 Breaking beer bottles with cavitation, SUNNY JUNG, Department of Mathematics, MIT, JAKE FONTANA, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University, MICHAEL SHELLEY. Courant Institute, New York University — Hitting the top of a beer bottle, nearly full of water, with an open hand can cause the bottle to break, with the bottom separating from upper section. We have studied this phenomenon using a high-speed camera, and observed the formation, coalescence and collapse of bubbles. The breaking of glass is due to cavitation, typically occurring near the bottom edge. We make numerical estimates of the relevant physical parameters, and compare these with experimental observations.

11:39AM B15.00003 Optical Tweezer as a Viscometer1, DANIEL ERENSO, SAMUEL ELROD, TAYLOR BARNES, ANTHONY FARONE, MARY FARONE, Middle Tennessee State University — An optical tweezer (OT) has been widely used to study the mechanical properties of microscopic living biological systems like red blood cells. These studies are based on measurement of deformations caused by a force exerted directly or indirectly by an optical trap. The trap is usually pre-calibrated using Stokes viscous force of the suspension fluids for the biological system which is directly proportional to the viscosity of the fluids. Therefore, calibration of the trap depends on the viscosity of the fluid which depends on temperature. In this work, we have demonstrated that OT can be used to precisely measure the viscosity of biological fluids affected by temperature. Using an infrared laser trap which is calibrated using silica sphere suspended in a distilled deionized water and measuring the power as function of escape velocity, we have measured the viscosities of a newborn and unborn bovine serum with a different concentration of antibodies.

1Daniel Erenso and Anthony Farone acknowledge support from FRCPC, and Taylor Barnes and Adam Shulman acknowledge support from URSCA at Middle Tennessee State University.
We therefore use an electrical method to probe viscous coalescence as early as 10 ns after contact. This technique was developed by Burton et al.\cite{1} transformation occurs as they rapidly coalesce into a single drop. Because of its speed and geometry, this finite time singularity is difficult to study optically.

12:03PM B15.00005 A Front Tracking Algorithm for Liquid Jet Breakup, \textbf{WURICEN BO, JAMES GLIMM, XINGTAO LIU} — A numerical study of breakup of a high speed jet is presented using the Front Tracking method in 3D. A robust locally grid based method is applied to handle the topological change of the surface mesh in the simulation, the validation of the method is proved mathematically. Numerical results are presented for 3D simulation of the primary breakup of a liquid jet with turbulent inflow.

12:15PM B15.00006 Coalescence and Pinch-Off in Viscous Liquids\cite{1}, \textbf{JOSEPH PAULSEN, University of Chicago, JUSTIN BURTON, Fred Hutchinson Cancer Research Center, SIDNEY NAGEL, University of Chicago} — When two fluid drops come into contact, a topological transformation occurs as they rapidly coalesce into a single drop. Because of its speed and geometry, this finite time singularity is difficult to study optically. We therefore use an electrical method to probe viscous coalescence as early as 10 ns after contact. This technique was developed by Burton et al.\cite{1} to study mercury drop pinch-off and adapted for salt-water coalescence by Case et al.\cite{2} revealing a breakdown of the expected universal dynamics in early-time inviscid coalescence. For viscous coalescence, we measure a resistance that decreases as $t^{-1}$ at early times and as $t^{-1/2}$ at late times, with a crossover time that increases with viscosity. In the inviscid case, these power laws had been interpreted with a model in which the drops coalesce at a slightly deformed interface.\cite{2} We explore this possibility as well as others, such as an anomalously long viscous regime. This electrical technique is also used to study viscous fluid pinch-off, which we compare with previous optical studies.\cite{1} J. C. Burton, J. E. Rutledge, and P. Taborek, Phys. Rev. Lett. 92, 244505 (2004). \cite{2} S. C. Case and S. R. Nagel, Phys. Rev. Lett. 100, 084503 (2008).\footnote{1This work was supported by the Keck Foundation, MRSEC, and NSF}

12:27PM B15.00007 Scaling Law for Driven Spreading and Coalescence of Sessile Droplets\cite{1}, \textbf{PILGUY KANG, SHAHAB SHOJAEI-ZADEH, CHRISTINE APPLEBY, SHELLEY ANNA, Department of Mechanical Engineering, Carnegie Mellon University, MICRO COMPLEX FLUIDS LABORATORY TEAM} — This study investigates the dynamics of spreading and coalescence of droplets on a surface, a process important in applications such as inkjet printing, spray coating, and flooding of fuel cells. We use a simple microfluidic device to control the spreading and merging processes. Droplet diameter and maximum height are monitored as functions of time. We compare the dynamics with existing scaling models modified to incorporate time independent demand, and we extend the model to describe the scaling behavior of the liquid bridge growing between merging droplets on a surface. The experiments agree well with the expected scaling.\footnote{1GuSH grant by Graduate Support Programs at Carnegie Mellon University}

12:39PM B15.00008 Temperature profiles near a pinned nucleating bubble, \textbf{SCOTT PARKER, CHANG-KI MIN, SUNG CHUL BAE, DAVID CAHILL, STEVE GRANICK, University of Illinois} — We have measured the temperature distribution on solid surfaces in contact with liquid jets and on the surface of the nucleating bubble using interferometry. Vapor bubbles butted by focused laser heating of an underlying metal substrate. Bubbles are pinned in place by suitable surface functionalization and their shape is characterized by interferometry. Varying the wettability of the surface to control the shape and surface lifetimes of bubbles, we have correlated contact angle, lift-off diameter, and local temperature.

12:51PM B15.00009 Effect of Encapsulated Polymers and Nanoparticles on Deformation of Droplets, \textbf{O. BERK USTA, University of Pittsburgh, DENNIS PERCHAK, Kodak US Research, ANDREW CLARKE, Kodak European Research, JULIA M. YEOMANS, Oxford University, ANNA C. BALAZS, University of Pittsburgh} — We investigate the effects of polymer chains and nanoparticles on the deformation of a droplet in shear and extensional flow using computational modeling. Our model accounts for both the solid and fluid phases explicitly. We show that under shear flow, both the nanoparticles and the encapsulated polymers reduce the shear-induced deformation of the droplet at intermediate capillary numbers. In contrast, under extensional flow we find that the long polymer chains inhibit the breakup and reduce deformation. We study the chain-length and concentration dependence and also present the effects of various parameters such as the wetting strength.

1:03PM B15.00010 Electrorheology Leads to Efficient Combustion, \textbf{R. TAO, Dept. of Physics, Temple University, K. HUANG, H. TANG, D. BELL, Temple University} — Improving engine efficiency and reducing pollutant emissions are important. Since combustion starts at the interface between fuel and air and most harmful emissions come from incomplete burning, reducing the size of fuel droplets for the fuel injection would increase the total surface area to start burning, leading to a cleaner and more efficient engine. While most efforts are focused on ultra-dilute mixtures at extremely high pressure to produce much finer mist of fuel for combustion, the new technique is still under development and only for next generation vehicles. Here we report our fuel injection technology based on new physics principle that proper application of electrorheology can reduce the viscosity of petroleum fuels. A small device is thus introduced just before the fuel injection for the engine, producing a strong electric field to reduce the fuel viscosity, resulting in much smaller fuel droplets in atomization. Both lab tests and road tests confirm our theory and indicate that such a device improves fuel mileage significantly and reduces emission. This technology is expected to have broad applications, applicable to current internal combustion engines and future engines as well. Supported by STWA and RAND.

1:15PM B15.00011 Evolution of Electrified Films on a Porous Inclined Plane, \textbf{UMA BALAKRISHNAN, University of California Santa Barbara, USHA RANGANATHAN, Indian Institute of Technology Madras} — The nonlinear stability of a thin conducting film flow down a porous inclined plane, while the electric field acts normal to the plane is considered. It is assumed that the flow through the porous medium is governed by Darcy’s law and the characteristic length of the pore space is much smaller than the depth of the fluid layer above. Integral Boundary Layer method is employed in obtaining a set of exact averaged equations for the flow film system. Linear stability results through normal mode analysis reveal that the destabilizing influence of the electric field is further enhanced by the porosity of the medium. Critical Reynolds number for the onset of instability decreases with the increase in the permeability of the porous plane. Weakly nonlinear stability analysis using method of multiple scales divulges the existence of zones due to supercritical stability and subcritical instability. Permanent finite-amplitude waves in the supercritical stable region are portrayed by solving the nonlinear evolution equation numerically in a periodic domain. The parameter ranges that support complex nonlinear dynamics is obtained through a combination of theoretical analysis and numerical experiments.
1:27PM B15.00012 Universal cone angle of ac electrosprays due to net charge entrainment, NISHANT CHETWANI, SIDDHARTH MAHESHWARI, H.C. CHANG, University of Notre Dame — The slender meniscus that is obtained by the application of high frequency AC field is quite distinct from DC Taylor Cone. This AC cone shows a continuous longitudinal growth and has much smaller half cone of ∼ 11°. Mass spectrometry on the microjet from the AC cone shows that dissociation reaction occurs at the tip but only the low- mobility anionic species are entrained to produce a charged cone. These free negative charges relax to the interface to produce a non-uniform surface charge density that scales with respect to the azimuthal radius as ρ^−1, to balance the singular normal capillary pressure. Repulsion of this entrained surface charge and the Maxwell pressure they induce are estimated with an elliptic integral and a variational formulation produces anomalous stress balance with capillary pressure that is only satisfied at a universal angle of 12.6° degrees for the liquids with high dielectric constant in good agreement with the measured values for the organic solvents used in experiments.

1:39PM B15.00013 Impact of Elasticity on Coating Flow near A Moving Contact Line, YULI WEI, STEPHEN GAROFF, Carnegie Mellon University, ENRIQUE RAMÉ, National Center for Space Exploration Research, LYNN WALKER, Carnegie Mellon University — The impact of fluid elasticity and shear thinning on the dynamic wetting of polymer solutions is important because many fluids, even those that are normally considered Newtonian, exhibit non-Newtonian behaviors in the high shear environment of the wedge-like geometry near a moving contact line. Even though this behavior is on the microscopic scale, it has significant impact on wetting on the millimeter scale. Shear thinning dramatically modifies the flow field near a moving contact line and results in a reduced curvature of the free surface. In this talk, we will focus on the effects due to fluid elasticity. Both experimental and theoretical results are presented. The fluids we use are the dilute solutions of high molecular weight polyisobutylene (PIB) which exhibit elasticity-dominated rheology with minimal shear thinning. Their wetting behaviors are compared to their oligomer “solvent,” which is considered Newtonian based on standard rheometry. We will also discuss a lubrication analysis of the wedge-like flow field using an Oldroyd-B constitutive relation to mimic the stress evolution of the elastic solution.

1:51PM B15.00014 Field-dependent thermal transfer in magnetic fluids, JUN HUANG, ZHENYU ZHOU, GEOFF HUSTON, WEBI LUO, Department of Physics, University of Central Florida — The temperature gradient across a quasi one-dimensional magnetic fluid was measured as a function of the magnetic field and field gradient. It was found that when the field gradient, VB, is anti-parallel to the temperature gradient, V T, the temperature gradient increases with increasing field and field gradient, but decreases for VB parallel to V T. For B and VB perpendicular to V T and gravity, the results are complex and depend on the local configuration of the field and field gradient. We will discuss the results in terms of the effect of local magnetic body force that originates from the local field and the local susceptibility on thermal transfer in magnetic fluids.

2:03PM B15.00015 How does the viscosity of a lubricant effect its tribological behavior? 1, M. AGGLETON, P. TABOREK, University of California, Irvine — The viscosity of many conventional lubricants varies by many orders of magnitude over a small temperature range. We have explored this variation to explore the effect of large viscosity changes on lubrication. We have used a sliding block tribometer to measure the coefficient of friction of a steel on steel system with a variety of vacuum compatible hydrocarbon lubricants. Each lubricant was thermally cycled in ultrahigh vacuum from room temperature to below the glass transition temperature. This varies the viscosity without changing the chemistry. Several theoretical models for the temperature dependence of the viscosity of hydrocarbons are applied. The theory described in Cameron (1981) is used to relate the change in viscosity to the coefficient of friction. Some lubricants are found to fit these models up to viscosities as high as 10⁶ centiStokes, while for others the model does not even qualitatively describe the data.

1This work is supported by Extreme Friction: MURI AFOSR # FA9550-04-1-0381.

Monday, March 16, 2009 2:30PM - 5:30PM — Session D14 DFD: Colloids II; Structure and Rheology 315

2:30PM D14.00001 Lock and Key Colloids 1, STEFANO SACANNA, WILLIAM IRVINE, PAUL CHAIKIN, DAVID PINE, NYU — We demonstrate a recognition mechanism between microscopic (colloidal) particles based on a simple “lock-and-key” principle that relies only on the complementary morphology of the particles involved. The system we developed consists of charge-stabilized spherical silica colloids (keys) and specially designed polymeric particles with spherical cavities (locks). The assembly of locks with keys is driven by depletion interactions between the particles and an uncharged water soluble polymer (poly-ethylene oxide). We show that by balancing electrostatic repulsion and depletion attraction, we induce a selective and reversible lock-and-key self-assembly. Moreover, we can design the lock and key single units to have separate functionalizables chemistries, such that the resulting composite particle (lock+key) will exhibit anisotropic surface properties.

1This work was supported by The Netherlands Organisation for Scientific Research (NWO).

2:42PM D14.00002 ABSTRACT WITHDRAWN —

2:54PM D14.00003 Pairwise Additivity in Colloidal Electrostatics, JASON W. MERRILL, Yale University, SUNIL K. SAINIS, Rowland Institute, ERIC R. DUFRENE, Yale University — We present a method for measuring electrostatic and hydrodynamic interactions between colloidal particles based on observations of short-time trajectories. We use this method to explore whether forces between colloidal particles can be considered pairwise additive by comparing the force between a pair of particles to forces between groups of several particles.

3:06PM D14.00004 Structure and dynamics of suspensions of nanoparticles in nematic liquid crystals, BRIAN GETTELFINGER, GARY KOENIG, JOSE MORENO-RAZO, University of Wisconsin, JUAN HERNÁDEZ-ORTIZ, Universidad Nacional de Colombia, NICHOLAS ABBOTT, JUAN DE PABLO, University of Wisconsin — A hierarchical modeling approach has been adopted to examine the structure and dynamics of nanoparticles suspended in liquid crystals. A molecular model is used to predict the defects that arise in nanoparticle assemblies, as well as their response to applied flow fields. The model is solved by resorting to a local basis function based technique. The validity of the model and our numerical results are established by direct comparison to results from molecular dynamics simulations of nanoparticles in nematic and isotropic liquid crystals. Results for particle diffusion and aggregation at equilibrium and in flowing systems are then used to interpret our experimental data for a variety of systems.
3:18PM D14.00005 Monodisperse polymethyl methacrylate (PMMA) spheres in organic media: synthesis update, ANDREW HOLLINGSWORTH, MARK ELSESSER, WILLIAM IRVINE, DAVID PINE, PAUL CHAIKIN, New York University — Since the publication of Antl, et al. [Colloids and Surfaces 17 (1986) 67–78] more than 20 years ago, several research groups in the soft condensed matter area have attempted the dispersion polymerization of sterically-stabilized PMMA particles. Most have found that success of this particular synthesis depends critically on the quality of the comb-graft stabilizer, poly(12-hydroxystearic acid)-g-PMMA. More recent work has extended the particle synthesis to include the incorporation of covalently attached, fluorescent dyes in the particle interior. Our goal has been to reproduce some of these results–a challenging task– and to improve the process, leading to a reliable method for preparing core-dyed PMMA particles. We will report on several important findings related to this research goal, and demonstrate that our particles can be used to make colloidal clusters via the recently published emulsion encapsulation and shrinkage technique [Science 301, 483–487 (2003)].

3:30PM D14.00006 A model nanocolloidal rod system to explore structural transitions in networks and bundles, GEORGINA WILKINS, University of Michigan, PATRICK SPICER, The Procter and Gamble Company, MICHAEL SOLOMON, University of Michigan — We introduce a model system consisting of self-assembled polyamide anisotropic colloids suspended in aqueous surfactant solutions. The colloidal particles are formed by precipitation from an amorphous polyamide powder that is dispersed with mechanical agitation in an aqueous surfactant phase at temperatures from 59 to 100°C. The aspect ratio increases monotonically with temperature: at T = 59°C, short rods with aspect ratio r = 8 ± 1 form. At T = 100°C, rope like structures with r = 306 ± 14 form. By confocal laser scanning microscopy (CLSM) and dynamic light scattering (DLS) as volume fraction is increased we show a structural transition from dilute rod behaviour with diffusive dynamics to a homogeneous network structure with increasingly slow dynamics. Furthermore, increasing the aspect ratio of rods induces the same structural transition from dilute rod behaviour to a network structure. Finally, we vary the interaction potential between the rods by a polymer induced depletion interaction and observe an unexpected quiescent network to bundle transition. The bundles are several rod diameters wide and 1 - 2 rod lengths long. The rods appear to be ordered nematically within each bundle. The bundling transition leads to an order of magnitude decrease in the storage modulus of the suspensions.

3:42PM D14.00007 Polymer grafted particles: Architectural effects on the dynamics, PANAYIOTIS VOUDOURIS, F.O.R.T.H., Heraklion, Greece, JIHOON CHOI, HONG DONG, Carnegie Mellon University, Pittsburgh, USA, GEORGE FYTAS, F.O.R.T.H., Heraklion, Greece, MICHAEL BOCKSTALLER, KRIS MATYJASZEWSKI, Carnegie Mellon University, Pittsburgh, USA — We present a combined static and dynamic light scattering study of two polystyrene PS&SiO

3:54PM D14.00008 Structure of Quasi-One Dimensional Ribbon Colloid Suspensions, BINHUA LIN, STUART A. RICE, The University of Chicago, THOMAS STRATTON, BIANXIAO CUI, Stanford University — We report the results of an experimental study of a colloidal fluid confined to a quasi-one dimensional (q1D) ribbon channel. Our findings confirm the principal predictions of previous theoretical studies of such systems. These are (1) that the density distribution of the liquid transverse to the ribbon channel exhibits stratification and (2) that even at the highest density the order along the strata, as measured by the longitudinal pair correlation function, is characteristic of a liquid.

3:40PM D14.00009 Dynamics of Internal Stresses and Scaling of Strain Recovery in Aging Colloidal Gels, AJAY SINGH NEGI, CHINEDUM OSUJI, Department of Chemical Engineering, Yale University — On cessation of flow, dilute suspensions of carbon black particles undergo rapid gelation and display instantaneous residual or internal stresses which relax slowly with time. We monitor the evolution of these stresses (under zero strain) and find a weak power law decay, σi\(\sim\)t\(^{-\gamma}\), over 5 decades of time where \(\gamma\approx0.1\). The system exhibits aging, with the elastic modulus scaling as a weak power law of elapsed time, \(G\sim\sigma_0 t^\beta\), with \(\beta\approx\alpha\). Imposition of zero stress conditions after waiting time \(t_w\), at internal stress \(\sigma_i(t_w)\), results in the recovery of the stress relaxation without the zero strain constraint. The system exhibits aging, with the elastic modulus scaling as a weak power law of elapsed time, \(G\sim\sigma_0 t^\beta\), with \(\beta\approx\alpha\). Imposition of zero stress conditions after waiting time \(t_w\), at internal stress \(\sigma_i(t_w)\), results in the recovery of the stress relaxation without the zero strain constraint. Older systems exhibit less recovery than younger ones. Remarkably, strain recoveries at different \(t_w\) can be shifted to construct a single master curve in which the magnitude of the recovery is shifted vertically according to \(\sigma_i(t_w)\) and horizontally simply with elapsed time. The scaling of the strain recovery of the internal stress state suggests that the internal stress state is characteristic of the age of the system and of the manner in which the system will continue to evolve. This result has important implications for our understanding of glassy behavior in soft materials.

3:38PM D14.00010 Synthesis and Self-assembly of Janus and Patchy Particles by Lift-up Microcontact Printing, SHAN JIANG, STEVE GRANICK, University of Illinois at Urbana and Champaign — Janus and patchy particles were synthesized by a simple and novel lift-up microcontact printing method. The geometry of the particles is revealed by both optical fluorescence microscopy and scanning electron microscopy. It is demonstrated that the Janus balance (geometry) of the particles can be easily fine tuned. Interesting and unique cluster structures were self-assembled from particles synthesized by this method. The method allows particles not only of divalent but also of trivalent geometry to be formed in large quantity.

3:36PM D14.00011 Thermal Properties of Particulate Suspensions, REBECCA CHRISTIANSON, JESSICA TOWNSEND, Franklin W. Olin College of Engineering — It has been known since the 1800’s that addition of solid phase particles to a liquid can improve the thermal conductivity of the liquid. However, the instability of such suspensions made them impractical for cooling applications. With the advent of affordable technology for synthesizing nanometer scale particles, it became possible for stable suspensions with improved thermal properties to be created. Initial investigations of nanoparticle suspension coolants (termed nanofluids) seemed to indicate an anomalous enhancement of the thermal conductivity above that predicted by conventional theories. However, subsequent experimental work showed issues with the reproducibility of these early results, which has been attributed by some sources to aggregation within the suspensions. We will present work from our group studying the properties and practical application of stable nanoparticle suspensions, as well as our initial findings on the effects of aggregation on the measured thermal properties of particulate suspensions.
4:54PM D14.00013 Adiabatic Intramolecular Movements for Water Systems in Ab initio simulations1. LUANA PEDROZA, ANTONIO J.R. DA SILVA, Physics Institute USP — The detailed description of hydrogen bonds in water is essential to understand the great variety of processes that occur in this system. Clearly the most appropriate way to do that description would be to treat all the degrees of freedom quantum mechanically. Another possibility is to treat the nuclei classically and the electrons quantum mechanically. A very common approximation in these simulations is to consider each water molecule as a rigid body, which clearly imposes a limitation on the real description of the molecules and their interactions. We here present an effective treatment of the intramolecular degrees of freedom of water, where these modes are decoupled from the intermolecular one, adiabatically allowing these coordinates to be positioned at their local minimum of the PES. This decoupling is performed combining an AIMC simulation using the rigid bodies approximation with an intramolecular optimization. As an application of our methodology we have studied small water clusters. We show that even in the case of the water dimer the sampling of phase space is significantly modified when intramolecular optimization is included (J. Chem. Phys., 128, 104311 (2008)). As a result, there are clear changes in features such as the dipole moment and structural properties.

1We acknowledge financial support from FAPESP and CNPq.

5:06PM D14.00014 New look of fractional exclusion statistics1, DRAGOS-VICTOR ANGHEL, Department of Theoretical Physics, Horia Hulubei National Institute of Physics and Nuclear Engineering — I discuss the concept of fractional exclusion statistics and I show that it leads to inconsistencies in the calculation of the Hilbert subspaces of particles in the system. In order to eliminate these inconsistencies, I introduce new mutual exclusion statistics parameters, which are proportional to the dimension of the Hilbert sub-spaces on which they act. These new definitions lead to properly defined particle distributions and thermodynamic properties. I also show that fractional exclusion statistics is manifested in general interacting systems and I calculate the exclusion statistics parameters. Most importantly, I prove that indeed, the mutual exclusion statistics parameters are proportional to the dimension of the Hilbert space on which they act.

Related publications:

5:18PM D14.00015 Capillary forces on nanowires, JUN MA, SHENFENG CHENG, Johns Hopkins University, JAY WALLACE, MACS Consulting, PATRICIA MCGUIGGAN, MARK ROBBINS, Johns Hopkins University — The capillary forces on nanowires have been measured by attaching them to the cantilever of an Atomic Force Microscope (AFM). The nanowires are immersed and retracted from a liquid/air interface. The entire capillary force curve is compared to continuum theory and molecular simulations. Nanowires with different diameters and chemistry and various liquids are investigated. Surface tension, contact angle hysteresis, and dynamical contact angles can be extracted under reasonable assumptions about how the contact line moves along the nanowires.

Monday, March 16, 2009 2:30PM - 4:54PM –
Session D15 DFD: Monolayers, Membranes and Microemulsions 316

2:30PM D15.00001 Nanoparticle–induced domain formation in zwitterionic lipid membranes, MEENAKSHI DUTT, ERIK LUIJTEN, University of Illinois at Urbana-Champaign — Charged nanoparticles have been found to induce coexistence of gel and fluid states in a pure zwitterionic membrane. The presence of the nanoparticle induces thermodynamic and structural changes in the model membrane. These changes are due to electrostatic interactions between the nanoparticle and the adjacent lipid monolayer. Analogies can be drawn between these systems and biological membranes, where domains in the vicinity of charged peripheral proteins play an important role in regulating cell activity.

To understand the differences in the structural and dynamical properties of coexisting domains in lipid membranes, we develop a coarse-grained model that represents the monolayer as a quasi two-dimensional plane of dipoles. The electrostatic interactions between the charged nanoparticle and the adjacent membrane monolayer, as well as the steric interactions within the monolayer, are incorporated explicitly. We will discuss our model and present results on the thermodynamic and structural changes in the model membrane induced by the presence of the nanoparticle.


2:42PM D15.00002 ABSTRACT HAS BEEN MOVED TO Y36.00013 –

2:54PM D15.00003 Langmuir films of chiral lipid molecules and Pattern Formation, PREM BASNET, ELIZABETH MANN, Dept. of Physics, Kent State University, Kent OH 44242, SAHRAOUI CHAIEB, Department Mechanical Science and Engineering, Bioengineering and the Beckman Institute University of Illinois at Urbana-Champaign, Urbana IL, 6180 — Langmuir films of 1,2-bis(10,12 Tricosadiynoyl)sn-Glycerol-3-Phosphoethanolamine form spiral and target patterns when compressed between two movable barriers in a Langmuir trough above 30°C, up to the chain-melting transition at ~37°C. The critical pressure, at which spirals appear, increases with temperature. The patterns themselves also depend on temperature, with single-armed spirals with many defects forming near 30°C and defect-free target patterns at higher temperatures. The mechanism of spiral formation could be a competition among elasticity, chirality, and the boundary conditions at the core of the domains. Optical anisotropy and the growth rate of internal structures test this suggested mechanism.

3:06PM D15.00004 Phase behavior of a binary phospholipid/cholesterol Langmuir monolayer: comparison of Brewster angle and fluorescence microscopy, FANINDRA BHATTA, PRITAM MANDAL, DAVID AL-LENDER, ELIZABETH MANN, Dept. of Physics, Kent State University, Kent OH 44242, YASMIN ISLER, Dept. of Chemistry, KSU, Kent OH 44242, EDGAR KOULJIAN, Dept. of Biology, KSU, Kent OH 44242, ANDREW BERNOFF, Dept. of Mathematics, Harvey Mudd College, Claremont, CA 91711 — The binary mixture of dihydrocholesterol and dimyristoyl phosphatidylcholine exhibits two liquid phases at the air/water interface: a cholesterol-rich and a phospholipid-rich phase, with a well-known critical point at a critical composition. Approaching that point with increasing monolayer pressure, the differences between phases disappear, along with the line tension between phases. In our experiments, the line tension is determined through comparison of the relaxation of domain shapes towards equilibrium with a compact, numerically tractable boundary integral model for the system hydrodynamics. We use both fluorescence microscopy and Brewster angle microscopy to visualize the lipid monolayer, and find the two methods have significant differences in monolayer behavior near the critical point.
3:18PM D15.00005 Large-scale free-standing monolayer membranes of nanoparticles: preparation and properties. JINBO HE, LASZLO FRAZER, James Franck Institute, University of Chicago, Chicago, Illinois 60637, USA, XIAO-MIN LIN, Materials Science Division, Chemistry Division and Center for Nanoscale Materials, Argonne National Laboratory, Argonne, Illinois 60439, USA, ADAM WEIS, HEINRICH JAEGGER, James Franck Institute, University of Chicago, Chicago, Illinois 60637, USA — Two-dimensional arrays of close-packed nanoparticles can be stretched across tens-micrometre-size holes. The resulting freestanding monolayer membranes extend over hundreds of particle diameters without crosslinking of the ligands or further embedding in polymer. In our previous results of dodecanethiol-ligated 6-nm-diameter gold nanocrystal monolayers, we find a Young’s modulus of the order of several GPa. This remarkable strength is coupled with high flexibility, enabling the membranes to bend easily while draping over edges. Recently we found that oleic-acid-covered cobalt nanoparticles (~9 nm in diameter) self-assemble at toluene/ethylene glycol interfaces and form large two-dimensional arrays. These membranes stretch across tens-of-micrometer holes after drying of ethylene glycol. The mechanical and diffusion properties of these membranes are tested and the response of these membranes under external fields is also investigated.

3:30PM D15.00006 Casimir force between inclusions in a stretchable fluid membrane. HSUANG-KU LIN, ROYA ZANDI, LEONID PRYADKO, Department of Physics, University of California at Riverside — We calculate the entropic fluctuational force, a finite-temperature analogue of the Casimir force, between foreign inclusions in a stretchable fluid membrane. Specifically, we consider the fluctuations of a planar membrane governed by the full Helfrich Hamiltonian, including the surface tension and both bending rigidity terms. The inclusions are introduced as circular regions where the surface tension and/or bending rigidities are modified from their values on the non-perturbed membrane. Results for arbitrarily-strong perturbations of the membrane, including holes, rigid disks, and edges will be presented.

3:42PM D15.00007 Breathable NIPAAm Network with Controllable Hydration Supports Model Lipid Membrane. MICHAEL JABLIN, HILLARY SMITH, MIKHAIL ZHERNENKOV, Lujan Neutron Scattering Center, AJAY VIDYASAGAR, RYAN TOOMEY, University of South Florida, JESSICA SAIZ, Lujan Neutron Scattering Center, BORIS TOPERVERG, Ruhr Universitat Bochum, ERIK WATKINS, TONYA KUHL, University of California, Davis, ALAN HURD, JAROSLAW MAJEWSKI, Lujan Neutron Scattering Center — The interaction of a model lipid bilayer composed of DPPC with a surface-tethered poly(N-isopropylacrylamide) (NIPAAm) was explored with neutron reflectometry (NR). The Langmuir-Blodgett / Langmuir-Schaeffer method was used to deposit a lipid bilayer onto the polymer. NR measurements were used to probe the in-and-out-of-plane structure of the system as a function of temperature. NR with fluorescence microscopy show that the polymer supports a lipid bilayer, and hydration of the support can be controlled. At low temp. the membrane develops out-of-plane undulations visible in off-specular scattering. Analysis of the off-specular reveals in-plane correlation of the bilayer fluctuations. The separation of the lipid bilayer from the solid support of a substrate constitutes a significant step towards a more realistic model of biological membranes.

3:54PM D15.00008 The effects of lung surfactant peptide mimic KL4 on lipid monolayer collapse. NIELS HOLTen-ANDERSEN, University of Chicago, Department of Chemistry, Chicago, IL 60637, USA, LUKA POCIvAVEK, University of Chicago, Department of Chemistry and James Franck Institute, Chicago, IL 60637, USA — We have investigated the origin of the positive effect of the peptide KL4 on lung surfactant lipid monolayers containing DPPC and POPG. Using surface balance techniques and fluorescence microscopy we have observed that KL4 rigidifies POPG containing lipid monolayers evidenced by a shift in their collapse mode. Rather than collapsing as a fluid by flowing into the sub-phase, a KL4 supported POPG monolayer instead collapses by folding. Furthermore, when KL4 is added to POPG containing monolayers they demonstrate an increased tolerance to repeated compression and expansion cycles while the opposite appears to be true for pure DPPC monolayers. We will discuss the potential role of electrostatic interactions in the rigidifying effect of KL4 on POPG containing monolayers in the context of the overall importance of collapse mode in establishing robust and reversible lipid monolayers.

4:06PM D15.00009 Microrheology of protein layers at the air-water interface. MYUNG HAN LEE, STEVEN CARDINALI, DANIEL REICH, Johns Hopkins University, KATHLEEN STEBE, University of Pennsylvania, ROBERT LEHENY, Johns Hopkins University — Due to their amphiphilic nature, many proteins in aqueous solution will adsorb at the air-water interface to create a viscoelastic interfacial layer. We present an investigation of the formation and mechanical properties of interfacial protein layers formed by beta-lactoglobulin using microrheological techniques including multiple particle tracking and magnetic nanowire microrheology. We observe the interfacial rheology evolve in time through three stages: (i) an increase in viscosity, (ii) a period of spatial heterogeneity in which the interface contains elastic and viscous regions, and (iii) the development of a uniformly rigid elastic film. We evaluate the dependence of this evolution on the protein-protein interactions, which we tune by varying solution pH. As we will discuss, these studies illustrate the power of microrheological approaches to interfacial rheology.

4:18PM D15.00010 ABSTRACT WITHDRAWN —

4:30PM D15.00011 ABSTRACT WITHDRAWN —

4:42PM D15.00012 Critical swelling of fluctuating capsules. HAIM DIAMANT, EMIR HALEVA, Tel Aviv University — In many natural transport processes the solute molecules to be transported are encapsulated in semipermeable, flexible membrane vesicles of micron size. We study the swelling of such fluctuating capsules, as the number of encapsulated particles is increased, or the concentration of the outer solution is decreased. The approach to the maximum volume-to-area ratio and the associated buildup of membrane tension involves a continuous phase transition and follow universal scaling laws. The criticality and its features are model-independent, arising solely from the interplay between volume and surface degrees of freedom.

8:00AM H14.00001 Connecting structure and rheology in sheared colloidal suspensions. JONATHAN MCCOY, ITAI COHEN, Cornell University — We investigate the shear properties of colloidal suspensions confined between parallel plates. When the distance between the plates is very small, i.e. approaching the size of the colloidal particles, a number of dramatic phase behaviors are observed under shear, including buckling, banding, jamming, and crystallization. This strongly confined regime is difficult to access using standard rheological techniques. Our experiment explores connections between microstructural behaviors and macroscopic flow by combining confocal microscopy and force measurement techniques in a custom-built thin-film shear cell. Here, we will focus on the interplay between confinement, slip, and order.

8:12AM H14.00002 Modulation of attractive colloidal interactions by lipid and protein membrane functionalization. YUPENG KONG, RAGHUVEER PARTHASARATHY, Univ. of Oregon, Dept. of Physics — The broad technological and scientific importance of colloidal materials has spurred a large body of research into the functionalization of micron-scale particles. Progress towards self-assembled monolayers (SAMs) for colloidal particles remains slow, however, and fundamental mysteries such as the attractive interactions observed between like-charged particles near a confining wall remain unresolved. These difficulties arise in large part due to the lack of experimental systems with tunable, attractive interparticle interactions. Biomembranes are appealing candidates for colloidal functionalization, enabling access to electrostatic and chemical properties that influence inter-particle relations. We describe here the first measurements of the pair interaction energy for membrane-functionalized colloids, using a newly developed optical line trapping technique. Two classes of particles, derivatized with lipid-only and lipid-plus-protein membranes, each show attractive interactions. The two particle types exhibit different relations between the depth and spatial range of the interactions, however. Control of lipid composition allows the first reported decomposition of like-charge interactions into charge-dependent and -independent terms, leading to a striking insight into the long-standing paradox of like-charge attraction: the dependence of the interaction is purely repulsive, while the attraction is independent of particle charge.

8:24AM H14.00003 Self-protected interactions in DNA-functionalized colloids: Nano Contact Glue. MIRJAM LEUNISSEN, Center for Soft Matter Research, New York University, REMI DREYFUS, ROUJIE SHA, NADRIAN SEEMAN, DAVID PINE, PAUL CHAIKIN — The ability of single-stranded DNA to form a variety of sequence-dependent secondary structures, such as hairpins, is frequently used in DNA nanotechnology, but has so far not been explored for the directed assembly of (nano)colloidal structures. We will show how mono- and bimolecular hybridization events in the DNA coatings of individual micrometer-sized beads can give rise to unusual, quench-rate dependent aggregation behavior, and how it can give additional control over the colloidal self-assembly process. For example, it provides us with ‘self-protected’ interactions that are activated by temperature or prolonged proximity and that facilitate the formation of finite-sized structures. A simple quantitative model describes the underlying competition between intraparticle and interparticle hybridization events, based on the known thermodynamic parameters of the DNA sticky ends.

8:36AM H14.00004 A simple quantitative model for the reversible association of DNA coated colloids. REMI DREYFUS, MIRJAM LEUNISSEN, ROUJIE SHAH, New York University, ALEXEI TKACHENKO, University of Michigan, NADRIAN SEEMAN, DAVID PINE, PAUL CHAIKIN, New York University — We investigate the reversible association of micrometer-sized colloids coated with complementary single-stranded DNA ‘sticky ends’ as a function of the temperature and the sticky end coverage. We find that even a qualitative description of the dissociation transition curves requires the inclusion of an entropic cost. We develop a simple general model for this cost in terms of the configurational entropy loss due to binding and confinement of the tethered DNA between neighboring particles. With this easy-to-use model, we demonstrate for different kinds of DNA constructs quantitative control over the dissociation temperature and the sharpness of the dissociation curve, both essential properties for complex self-assembly processes.

8:48AM H14.00005 Observation of condensed phases of quasi-planar core-softened colloids. PRIMOZ ZIHERL, University of Ljubljana & Jozef Stefan Institute, NATARAN OSTERMAN, DUSAN BABIC, IGOR POBERAJ, University of Ljubljana, JURE DOBNIKAR, Jozef Stefan Institute — We experimentally study the condensed phases of repelling core-softened spheres in two dimensions. The dipolar pair repulsion between superparamagnetic spheres trapped in a thin cell is induced by a transverse magnetic field and softened by suitably adjusting the cell thickness. We scan a broad density range and we materialize a large part of the theoretically predicted phases in systems of core-softened particles, including expanded and close-packed hexagonal, square, chain-like, stripe/labyrinthine, and honeycomb phases. Further insight into their structure is provided by Monte Carlo simulations.

9:00AM H14.00006 In situ real time measurement of temperature responsive nanoparticles. DENIS PRISTINSKI, THOMAS Q. CHASTEK, VIVEK PRABHU, KALMAN MIGLER, Polymers Division, NIST — In this work, we combine dynamic light scattering (DLS) and diffusing wave spectroscopy (DWS) to evaluate the size of temperature responsive nanoparticles over a broad range of concentrations. A fiber optic probe DLS instrument was previously demonstrated to measure nanoparticle solutions at a relatively high concentration. The incorporation of back-scattering DWS further extends the technique application to highly turbid conditions. The combined setup was designed to have a simplified and compact optical arrangement employing singlemode fiber based components. Data analysis for both methods was carried out using integrated open source cross-platform software. Measurements were conducted to monitor the progress of poly(N-isopropyl acrylamide) nanoparticle syntheses, including a multi-step cross-linking step. Measurement were done in a custom-built thin-film shear cell. Here, we will focus on the interplay between confinement, slip, and order.

9:12AM H14.00007 Enhanced particle transport in an oscillating sinusoidal optical potential. WEIQIANG MU, Northwestern University, LAN LUAN, Northwestern University, GANG WANG, Indiana University, Purdue University, Fort Wayne, GABRIEL SPALDING, Illinois Wesleyan University, JOHN KETTERSON, Northwestern University, NORTHWESTERN UNIVERSITY COLLABORATION, INDIANA UNIVERSITY, PURDUE UNIVERSITY, FORT WAYNE COLLABORATION, ILLINOIS WESLEYAN UNIVERSITY COLLABORATION — We have studied the delivery of a colloidal particle in the presence of an oscillating, spatially periodic, optical potential. The average particle velocity relative to the fluid velocity in this potential depends greatly on the oscillation amplitude and frequency. The results of both our simulations and experiments show that for some combinations of these parameters, the average particle velocity can be enhanced due to the synchronization of the particle movement with the oscillating potential.

9:24AM H14.00008 Charge inversion in monovalent ionic solutions. ALEX TRAVESSET, Iowa State University and Ames Lab, ALBERTO MARTIN-MOLINA, Universidad de Granada, CARLES CALERO, IORDI FARAUDO, Institut de Ciencia de Materials de Barcelona, MANUEL QUESADA-PEREZ, Universidad de Jaen, ROQUE HIDALGO-ALVAREZ, Universidad de Granada — We present measurements of the mobility of colloids as a function of the concentration of the monovalent salt Tetraphenyl Arsonium Chloride (TACl). The experiments show a decrease of the mobility with increasing salt concentration that flips sign (charge inversion) at mM salt concentrations. A modified version of the O’Brien and White theory taking into account the hydrophobic nature of the phenyl groups describes the experimental data without fitting parameters. Saturation effects in the mobility as well as possible generalizations are also discussed.
9:36AM H14.00009 Position Control of Particles embedded in Microbeads and Fibers Produced by Electrohydrodynamics.¹, UNYONG JEONG, EUN MIN JO, SUNGWON LEE, KYU TAE KIM, Department of Material Science and Engineering, Yonsei University, Seoul, Korea — Electrohydrodynamics is a good approach to produce uniform-sized colloids and fibers in a continuous process. The dimension can be controlled from tens of nanometers to a few micrometers. The structure of the colloids and nanofibers from electrohydrodynamics has been diversified according to the uses. Especially, core-shell structure and hybridization with functional nanomaterials are fascinating due to their possible uses in drug-delivery systems, multifunctional scaffolds, organic/inorganic hybrids with new functions, and highly sensitive gas- or bio-sensors. This talk will present the structural variations by tuning the position of small particles in the colloids and fibers produced from electrohydrodynamics and demonstrate their possible applications.

¹This work was supported in part by KOSEF grant (No. R01-2007-001-11281-0) funded by MOST and Seoul R&BD Program (10816).

9:48AM H14.00010 Using colloids to model atomic thin film growth. RAJESH GANAPATHY, MARK BUCKLEY, ITAI COHEN, Cornell University — We epitaxially grow colloidal thin films by sedimenting micron sized colloidal particles on a microfabricated substrate. The attractive interaction between the colloids, induced by a depletant polymer, leads to the nucleation of islands that grow and coalesce with one another. We use confocal microscopy and particle tracking to study the dynamics of the colloidal particles as they diffuse, aggregate and rearrange configurations during deposition. The saturation island density is estimated as a function of the deposition rate and depletant concentration. We find that our results are in excellent agreement with those obtained from atomic deposition experiments suggesting that our system can be used to model various phenomena that occur in atomic thin film growth. Furthermore, we quantify the Ehrlich-Schwoebel step edge barrier by using holographic optical tweezers to create artificial islands and study the dynamics of colloidal monomers placed on the edge of these islands. Owing to the short-range of the attractive interaction in our system, the origin of the step edge barrier in colloids is strikingly different from atoms.

10:00AM H14.00011 Stochastic Rotational Dynamics Simulations of Nanocolloid Suspensions², JEREMY B. LECHMAN, MATT K. PETERSEN, STEVEN J. PLIMPTON, P. RANDALL SCHUNK, GARY S. GREST, Sandia National Laboratories, PIETER INT VELD, Polymer Research, BASF — The use of nanoparticle suspensions to potentially tailor the functionality of composite devices has broad applicability, but is limited in practice, in part, due to poor understanding of the phenomena at that scale. In order to address this we have implemented a mesoscale fluid technique called Stochastic Rotation Dynamics (SRD). Here, we discuss the use of this method to investigate the behavior of hard sphere like nanocolloids. In particular we will present a direct, “one-to-one” comparison of an SRD fluid with an explicit Lennard Jones solvent. For small colloids in this low viscosity fluid no “telescoping of timescales” is required for efficiency, which allows us to consider the accuracy of the base numerical scheme without complicating approximations. We present the diffusion and reduced viscosity as a function of volume fraction of colloids and compare to well known results. The efficiency of an SRD simulation relative to an explicit atom simulation is also discussed.

²Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract No. DE-AC04-94AL85000.

10:12AM H14.00012 Light-induced structure transformation of colloidal nanocrystals by using generalized Ewald-Kornfeld formulation¹, M.J. ZHENG, K.L. CHAN, K.W. YU, The Chinese University of Hong Kong — When metallic nanoparticles are brought close together and they are illuminated by laser light, there will be strongly enhanced forces between these particles [1]. If these particles are suspended in a liquid, the force can promote aggregation. As a result, the cluster size can exceed the wavelength of light and retardation effect must be considered. For this sake, we derived a generalized Ewald-Kornfeld summation [2] which is valid for fully retarded electromagnetic interaction. More importantly, we have extended the formula for a many-point basis in a unit cell. We used the formula to study the colloidal nanocrystal formation and transition driven by surface plasmon resonance enhanced forces. Our results are of fundamental importance to the relevant topics in soft matter physics and can be widely applied in the research of light-induced manipulation.


¹Work supported by the General Research Fund of the Hong Kong SAR Government

10:24AM H14.00013 Universal Nanocolloid Deposition Patterns: Harmonics of a Taylor Cone and Separation of DNA-Hybridized Nanocolloids¹, XINGUANG CHENG, HSUEH-CHIA CHANG, University of Notre Dame — With judiciously placed far-field electrodes, harmonics of the Laplace equation are selected near a conducting Taylor cone with discrete polar angles for the field maxima. Charged nanocolloids ejected along the discrete electric field lines of these mode maxima are observed to deposit a universal spectrum of rings on an intersecting plane, with particles of different size occupying different spectral lines due to different residue charge. After an affine transformation, nanocolloids ejected into a microslit and deposited onto one substrate exhibit the same universal line spectra. The size-selective deposition pattern is used to quantify DNA hybridization yield onto oligo-functionalized nanocolloids.

¹This work was supported by the DTRA (HDTRA1-08-C-0016).

Tuesday, March 17, 2009 11:15AM - 1:27PM
Session J14 DFD: Jammed Particles 315

11:15AM J14.00001 Porosity of mixed granular media of hard and soft grains, EMILIE VERNEUIL, DOUGLAS J. DURIAN, University of Pennsylvania — The addition of soft particles to granular materials modifies the packing properties such as the volume fraction and the interconnection of pores as a consequence of the particles stiffness. A macroscopic property that depends on the local arrangement of the grains is the hydraulic conductivity. Hence, hydrogel particles are developed as additives to sandy soils to improve the irrigation efficiency by decreasing the rate of far depth infiltration. However the parameters that control the mixed material porosity have not been explored. Our experimental study of the flow properties of mixtures of glass beads and swollen hydrogels aims at deriving simple arguments to connect the macro-scale measurement of the hydraulic conductivity to the arrangement of the grains around the soft particles, which determines the fraction of blocked pores. Our results show that the porosity decreases with the number of swollen gel per unit volume of the mixture. The conductivity also decreases as the size ratio of gel to glass bead decreases down to 1. A simple description accounting for the elastic contacts between glass beads and gel surface qualitatively accounts for the data.
11:27 AM J14.00002 Experimental characterization of microstate probabilities in mechanically stable packing of frictionless disks. M.D. SHATTUCK, Levich Institute and Physics Department, The City College of New York, New York, NY, C.-J. GAO, Department of Mechanical Engineering, Yale University, New Haven, CT, J. BLAAUWZDIEWICZ, C.S. O’HERN, Departments of Mechanical Engineering and Physics, Yale University, New Haven, CT — We report on a new experimental technique to produce mechanically stable packings of frictionless disks. The system consists of a quasi-2D vertical cell filled with bi-disperse disks. The disks are vigorously shaken and then allowed to settle under gravity in the presence of high-frequency low-amplitude vibrations to eliminate frictional effects. For a system of $T$ particles we find approximately 1000 mechanically stable states. The most probable states occur at least $10^9$ times more often than those that are least probable. This is in direct contradiction to the fundamental postulate in statistical mechanics, that all possible microstates are equally probable and calls into question granular theories based on this assumption. We have measured the frequency distribution of the states in the experiments and in corresponding discrete element simulations, and find excellent agreement. We have also examined how the microstate distribution scales with system size and will connect the microstates to macroscopic quantities such as the density to predict the statistics of macroscopic properties.

11:39 AM J14.00003 Spectral responses in granular compaction, LING-NAN ZOU, The James Franck Institute and Department of Physics, the University of Chicago — I study the compaction of a granular pack under periodic tapping. The magnitude of acceleration $\Gamma$ at each tap is modulated with frequency $\omega$ and amplitude $\delta \Gamma$: $\Gamma(t) = \Gamma_D C \sin(\omega t)$. The phase lag between $\Gamma(t)$ and $v(t)$ is denoted by $\delta \Gamma$. As a function of $\Gamma_D$, $\chi'_s(\omega)$ and $\chi'_s(\omega)$ are peaked at low $\Gamma_D$, a behavior reminiscent of the temperature-dependent susceptibilities in dielectric and spin glasses. For the packing of small particles ($d = 0.5$ mm) in ambient pressure, $\chi'_s(\omega)$ exhibits memory and rejuvenation effects under $\Gamma_D$ cycling, similar to that seen in the magnetic susceptibility of spin glasses when subjected to thermal cycling [1]. However this memory effect is suppressed for the packing of larger particles and in vacuum. The measurement of volume susceptibilities shows promise as a new way to study the packing of granular materials, and as an avenue to explore analogies between jammed grains and molecular and spin glasses.

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This work is supported by NSF and MRSEC.

11:51 AM J14.00004 Deformed Droplets in Static Two-Dimensional Emulsions, PEARL J. YOUNG, DANDAN CHEN, ERIC R. WEEKS, Physics Dept., Emory University — We confine oil-in-water emulsions between two parallel plates, so that the droplets are essentially squeezed into quasi-two-dimensional disks, somewhat analogous to granular photoelastic disks. By varying droplet area fraction, we seek to quantify the jamming transition of this static system. At a critical area fraction, the composition of the system should no longer be characterized primarily by circular disks but by disks deformed to varying degrees. We study a system of toluene droplets in water. As expected, we find that an increase in area fraction corresponds with an increase in average droplet deformation. Further, an increase in average droplet deformation corresponds with an increase in the heterogeneity of deformation within a given sample.

12:03 PM J14.00005 Jamming of Rod-like Granular Materials in Hoppers, SUMMER SARAF, SCOTT FRANKLIN, Rochester Institute of Technology — Long thin rods form solid plugs that are far more rigid than piles of ordinary sand, greatly affecting their ability to flow through small openings. We have built a hopper whose aperture, angle, and width can be independently varied and are studying the frequency with which rods of different length, width, and aspect ratio jam. As the opening aperture becomes larger, the mean number of particles that exit the hopper before a jam occurs naturally increases, but the probability distribution of fluctuations about this mean is unchanged. Unexpectedly, whereas the event distribution function $P(a)$ for spheres decays exponentially, we find the distribution for rods falls off as a power law with exponent $-1.41 \pm 0.08$. We are also investigating the growth of the mean event size $a_0$, as the aperture increases for possible divergence, which would imply a critical aperture size above which particles would never jam.

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This experiment supported in part by grants from the Research Corporation and the National Science Foundation.

12:15 PM J14.00006 Forces and displacements near the granular jamming threshold, MAHESH BANDI, Los Alamos National Laboratory, ANDRAS LIBAL, University of Antwerp, MICHAEL RIVERA, ROBERT ECKE, Los Alamos National Laboratory — We experimentally study the dynamics of jamming by dragging a probe disk in a two-dimensional bi-dispersed system of randomly packed photo-elastic disks. All measurements are made at packing fractions relative to the critical fraction at which jamming occurs. We measure the local force felt by the probe disk and compare it with the system’s global response with sensors placed along the system boundaries. We also visually monitor the disk displacements in the system, which are expected to be increasing constraints as a function of increasing packing fraction.

12:27 PM J14.00007 The angoricity describes the approach to the jamming, KUN WANG, CHAOMING SONG, PING WANG, HERNAN MAKSE, Levich Institute and Physics Department of CCNY — The application of concepts from equilibrium statistical mechanics to out of equilibrium systems has a long history offering the fascinating possibility to describe a diverse range of systems from glasses to grains. For jammed systems, the key idea was to replace the energy ensemble describing conservative systems by the volume ensemble for dissipative jammed systems. However, this approach is not able to describe the jamming critical point for deformable particles such as emulsions where the volume fraction, coordination number and elastic moduli behaves as power-law of the external stress as the system approaches jamming. The geometrical considerations have to be augmented by the ensemble of stresses described by the angoricity which replaces the role played by the temperature in thermal systems. Here we perform a basic test of the stress ensemble of jammed matter by following two independent approaches: we exhaustively enumerate the available jammed states and numerically follow the dynamics of the system near the jamming point. A direct comparison between both methods supports the idea of thermalization at a given angoricity which is shown to determine the systems state as it approaches the jamming transition. This result opens the possibility to calculate important quantities near $J$-point.

12:39 PM J14.00008 Equilibration in model granular subsystems: An experimental test for Edwards’ compactivity, FREDERIC LECHENAULT, JAMES PUCKETT, KAREN DANIELS, NCSU — We experimentally investigate the statistical features of the stationary states reached by two idealized granular liquids able to exchange volume. The system consists in two binary mixtures of the same number (and area) of soft disks, but with different surface properties. The disks sit on a horizontal air table and are separated by a mobile wall. Energy is injected in the system by means of an array of randomly activated coil bumpers standing as the edges of the cell. Due to the energy injection, the system acts as a mixture of soft disks, but with different surface properties. The disks sit on a horizontal air table and are separated by a mobile wall. Energy is injected in the system by means of an array of randomly activated coil bumpers standing as the edges of the cell. Due to the energy injection, the system acts like a slow liquid and eventually jams at high packing fraction. We characterize the macroscopic states by studying the motion of the piston. We find that its average position is different from one half, and is a non monotonic function of the overall packing fraction, which reveals the crucial role played by the surface properties in the corresponding density of states. We then study the bulk statistics of the packing fraction and find confirmation of the macroscopic behavior. However, the local fluctuations of the packing fraction are uniquely determined by its average, and hence independent of the interaction between disks. This result, together with the existence of a point at which the two sub-systems have the same volume, enables us to show that Edwards’ compactivity does not have the same value in the two equilibrated subsystems.
The work of MM and BC has been supported by NSF DMR-0549762 and The work of CS and CO has been supported by CDR-0835742 (CS) and DMR-0418838 (CSO).

1Supported by USDOE, AFOSR, and NSF.

2:06PM L6.00002 Flows and jets around compact astrophysical objects, JOHN HAWLEY, University of Virginia — No abstract available.

3:42PM L6.00003 Fluid Mechanics of the Geodynamo, PETER OLSON, Johns Hopkins — Fluid dynamical processes in the molten, iron-rich, electrically conducting core sustain Earth’s magnetic field. Convection driven by secular cooling and chemical differentiation is the primary energy source for the geomagnetic field. Earth’s rotation imparts helicity to the convection, which amplifies the geomagnetic field, balancing losses from Ohmic dissipation. Both the Ekman and Rossby numbers are very small in the outer core, so the convection is partly aligned with the planetary spin axis, which tends to orient the geomagnetic dipole axis in the north-south direction. The magnetic Reynolds number in the outer core is about 20 times the critical value for sustained dynamo action and the Reynolds number is about 10^{17}, implying turbulent conditions. Fluctuations in the turbulence induce continuous changes in the geodynamo field, including occasional polarity reversals. Geomagnetic polarity reversals have occurred about once every 250 kyr on average over the past 5 Myr, the last reversal occurred around 780 ka and there have been several long constant- polarity superchrons. The axial dipole collapses before a reversal, exposing the complex non-dipolar transition field, then the axial dipole is regenerated in the opposite polarity, the entire process lasting 10-20 kyr. Spontaneous polarity reversals have been observed in at least one liquid sodium dynamo experiment. Downward-extrapolated measurements from Earth-orbiting satellites reveal the axial dipole comes mostly from a few high-latitude concentrated flux spots on the core boundary. About 15% of the core boundary has reversed-direction magnetic field, mostly in the southern hemisphere. Proliferation and growth of reversed flux regions are major reasons why the axial dipole is in decline, decreasing at 10 times its free decay rate and suggesting (to some) that the geomagnetic field may be in early stage of a polarity reversal.

4:18PM L6.00004 Statistics and scaling in magnetohydrodynamic turbulence, WOLF-CRISTIAN MÜLLER, Max-Planck-Institut für Plasmaphysik, 85748 Garching, Germany — The nonlinear cascade of energy is one of the most prominent processes in turbulent systems. The associated self-similarity of two-point statistics leads to the appearance of inertial-range scaling laws, e.g. in the energy spectrum of turbulence. The scaling exponents that are observed in experiments or direct numerical simulations allow to verify the validity of cascade phenomenologies. Currently, controversial findings have led to a confusing situation in the phenomenological understanding of nonlinear inertial-range dynamics of magnetohydrodynamic turbulence which is discussed using recent results of direct numerical simulations. A new approach for investigating turbulent nonlinear dynamics which is based on the Lagrangian description of turbulence is also presented.
Tuesday, March 17, 2009 2:30PM - 5:30PM – Session L14 DFD: Colloids IV: Colloids and Interfaces

2:30PM L14.00001 The equilibrium colloidal crystal/colloidal liquid interface, ERIC R. WEEKS, JESSICA HERNANDEZ-GUZMAN, Physics Dept., Emory University — We use confocal microscopy to study an equilibrated crystal-liquid interface in a colloidal suspension. The surface shows spatial fluctuations due to capillary waves. Local measurements of the structure and dynamics near the rough surface reveal that the intrinsic surface, while meandering in space, is locally sharply defined. Examining different quantities finds slightly different widths of this intrinsic surface.

In terms of the particle diameter \( d \) and the intrinsic surface, while meandering in space, is locally sharply defined. Examining different quantities finds slightly different widths of this intrinsic surface.

2:42PM L14.00002 Janus particles at the liquid-liquid interface, QIAN CHEN, STEPHEN ANTHONY, STEVE GRANICK, University of Illinois Urbana Champaign — Dipolar Janus particles (negatively charged on one side, positively charged on the other), deposited on PDMS droplets in water, are studied in real time by fluorescence and phase contrast microscopy. Crystals form, under some conditions with long-range hexagonal order, but this self-assembled structure depends strongly on particle size and ionic strength of the water phase. Their provocative translational and rotational dynamics is studied using single-particle tracking.

2:54PM L14.00003 Short-time self-diffusion of nearly hard spheres at an oil-water interface, PENG TONG, YUAN PENG, WEI CHEN, Department of Physics, Hong Kong University of Science and Technology, THOMAS FISCHER, Institute of Experimental Physics V, University of Bayreuth, DAVID WEITZ, Department of Physics and School of Engineering and Applied Sciences, Harvard University — Optical microscopy and multi-particle tracking are used to study hydrodynamic interactions of monodisperse polymethylmethacrylate (PMMA) spheres at a decalin-water interface. The short-time self-diffusion coefficient measured at low surface coverage has the form, \( D_2^S(n) = \alpha D_0(1 - \beta n) \), where \( n \) is the area fraction occupied by the particles and \( D_0 \) is the Stokes-Einstein diffusion coefficient in the bulk suspension of PMMA spheres in decalin. The measured values of \( \alpha \) are found to be in good agreement with the numerical calculation for the drag coefficient of interfacial particles. The measured values of \( \beta \) differ from that obtained for bulk suspensions, indicating that hydrodynamic interactions between the particles have interesting new features at the interface.

1Work supported by the Research Grants Council of Hong Kong SAR.

3:06PM L14.00004 Observing the three-dimensional motion of colloids at an oil-water interface, RYAN MCGORTY, DAVID KAZ, Harvard University, SHANKAR GHOSH, Tata Institute of Fundamental Research, V.N. MANOHARAN, Harvard University — Our experimental system allows us to place micron-sized colloids at a flat oil-water interface. Using digital holographic microscopy we track the motion of particles at the interface in all three dimensions. Of particular interest is the out-of-plane motion of an adsorbed particle. I will present data of such motion and what it reveals regarding the energy and length scales of a particle attached to an interface. Introducing a laser tweezier and customized colloids (such as core-shell particles) into our experiment allows us to further investigate this system.

3:18PM L14.00005 Self-assembled Capillary Arrows, JEAN-CHRISTOPHE LOUDET, BERNARD POULIGNY, Centre de Recherche Paul Pascal, CNRS 115 avenue A. Schweitzer 33600 Pessac, France — Anisotropic particles adsorbed at a water-air interface are known to aggregate due to capillary interactions. We show that the packing configuration of a pair of prolate ellipsoids critically depends on their relative size and/or aspect ratio mismatch. While identical particles simply pack side-by-side, particles of slightly different sizes are observed to systematically self-assemble into characteristic arrows, i.e. with a finite angle between their axes. The occurrence of such arrows cannot be explained within the far-field approximation of interacting polar quadrupoles. A numerical analysis is worked out which allows us to explore the near-field characteristics of the capillary interaction. Results clearly show the destabilization of the side-by-side configuration due to a size mismatch, in agreement with experimental observations.

3:30PM L14.00006 Impact of Surfactant Sorption Kinetics on Microscale Tipstreaming, WINGKI LEE, LYNN WALKER, SHELLEY ANNA, Carnegie Mellon University — A microfluidic flow focusing system has been used to synthesize submicron sized droplets via a thread formation mode of drop breakup. This process utilizes the interaction of fluid motion and surfactant transport to draw out a thin thread, which then fragments into a stream of tiny droplets whose sizes are orders of magnitude smaller than the size of the device. In this work, we use a homologous series of \( C_n \) Es (\( n = 10, 12 \) and 14) surfactants to probe the impact of surfactant sorption kinetics on this process. To characterize the effects of these surfactants on the thread formation process, we measure the relevant timescales for the formation of a cone-like interface, the drawing and disintegration of a fine thread, and the period with which the process repeats. We then relate these timescales to the characteristic timescales for transport of surfactants to the oil-water interface. These measurements and simple scaling analyses suggest ways to extend the thread length and optimize the overall yield of submicron droplets.

1This research was supported by the National Science Foundation Grants Nos. CBET-0608864 and CBET-0730727. Acknowledgement is made to the Donors of the American Chemical Society Petroleum Research Fund for partial support of this research.

3:42PM L14.00007 Network Formation at the Air-Water Interface, ALINE MILLER, MARIA SIMON SAENZ DE SAMANIEGO, University of Manchester — A series of diacetylene end functionalised peptides have been designed to form beta-sheet rich monolayers at the air-water interface and their structure, rheological properties and ability to polymerize in response to UV light have been studied using a Langmuir trough and dilatational rheology. Surface pressure-area isotherms as well as compression-expansion cycles reveal all our peptide monolayers organise into the three distinct organisational states typically observed for surfactants at the air-water interface: gaseous (G), liquid expanded (LE) and liquid condensed (LC) and the limiting area per molecule suggests the alternating amphiphilic character of the peptide causes the molecule to orient with its long axes parallel to the air-water interface. The presence of the diacetylene group enhances surface activity and stability over time. Here we will discuss how peptide sequence, UV exposure strength and time, as well as peptide concentration (and hence organisation) influence the kinetics of network formation, and the morphology and mechanical properties of the final network formed.
4:06 PM L14.00009 Structures formed by colloidal particles on a droplet at small particle number. JEROME FUNG, RYAN J. MCGORTY, Harvard University, Dept. of Physics, VINOTHAN N. MANOHARAN, Harvard University, Dept. of Physics and SEAS — We discuss 3D imaging studies of the self-assembled structures formed by small numbers (N ~ 10) of micron-sized polymethylmethacrylate (PMMA) colloids pinned to the surface of a ~10 micron oil droplet in an aqueous solution. In the low N limit, these structures are governed by the interactions between the constituent colloidal particles on a given droplet. We prepare these droplets using a capillary microfluidic device. Since the droplets are not density matched to the continuous phase, we study them with a time-averaged zero gravity apparatus, based on a rotary stage. Specifically, we image the 3D structures formed by the colloidal particles on the droplets using digital holographic microscopy (DHM). DHM records the 2D interference patterns, or holograms, formed by light scattered from the colloidal particles and unscattered light. Subsequent analysis of the holograms, based on the Lorenz-Mie solution for light scattering by spheres, allows us to determine the 3D particle positions with time resolution limited by the camera frame rate.

4:18 PM L14.00010 Interfacial rheology in complex flow. JEFFREY MARTIN, STEVEN HUDSON, National Institute of Standards and Technology — Multiphase liquid systems are omnipresent in and essential to everyday life, e.g., foods, pharmaceutics, cosmetics, paints, oil recovery, etc. The morphology and stability of such systems depend on dynamic interfacial properties and processes. Typical methods utilized to measure such interfacial properties often employ drops that are much larger and flows that are much simpler than those encountered in typical processing applications. A microfluidic approach is utilized to measure dynamic structure and kinetics in multiphase systems with drop sizes comparable to those encountered in applications and flow conditions. The complex rheology of viscoelastic droplets in clear mineral oil is measured using particle tracers and a detailed shape analysis, which is capable of measuring sub-micron deviations in drop shape. Deformation dynamics, detailed drop shape, interfacial tension, and internal circulation patterns and velocities are measured in Poiseuille and transient elongational flows. Flow kinematics are adjusted by varying the microchannel geometry, drop size, and drop height. The effects of confinement on interfacial dynamics and circulation patterns and velocities are also explored.

4:30 PM L14.00011 Reverse coffee-ring effect. BYUNG MOOK WEON, LEI XU, Department of Physics, School of Engineering and Applied Sciences, Harvard University, JUNGHO JE, X-ray Imaging Center, Department of Materials Science and Engineering, Pohang University of Science and Technology, YEUKUANG HIU, Academia Sinica, GIORGIO MARGARITONDO, Ecole Polytechnique Fédérale de Lausanne, DAVID A. WEITZ, Department of Physics, School of Engineering and Applied Sciences, Harvard University — When a coffee drop dries on a solid surface, it commonly leaves a ring-like deposit along the edge, known as the coffee-ring effect. We present a reverse motion of particles in drying droplets, opposite to the coffee-ring effect. We reveal that the particle motion, initially toward the edge by the typical coffee-ring effect, is reversed to the droplet center owing to the capillary interaction generated by the droplet surface. The reverse coffee-ring effect always occurs whenever the capillary interaction prevails over the net outward force by the coffee-ring effect. The interaction predicts an inverse power-law time growth of moving distance from the edge, depending mostly on particle size and contact angle. The reverse coffee-ring effect may contribute to multiple ring formation by sweeping particles toward the center. We prove the mechanism with real-time optical, confocal, and X-ray microscopic observations of colloidal fluids.

4:42 PM L14.00012 Measurements of contact forces at the bottom of a droplet pile. HAO WANG, Department of Physics, University of Massachusetts Amherst, T. PRISK, J. ZHOU, A. DINSMORE — We measure the contact forces at the bottom of a container of frictionless liquid droplets as a function of compression and of distance to the container wall. Glass cylinders are used to contain 20-micron-radius droplets of silicon oil. Brownian motion is not significant for this size. Reflection interference contrast microscopy is used since we are particularly interested in contacts with the bottom surface. By looking at the Newton’s Ring interference pattern, we measure the deformation of each droplet, which arises from gravity and pressure from the whole pile transmitted through droplet contacts. We also measure the radius of each droplet and thereby obtain the vertical contact force. We vary the pile height to change the compressive stress and then measure the corresponding forces, probability distributions, and correlations of rearrangements. The results elucidate the roles that friction and confining walls play in granular systems and also shed light on force chains in bulk of the material.

4:54 PM L14.00013 Sticking colloids to liquid-liquid interfaces one by one. DAVID KAZ, RYAN MCGORTY, Harvard University, SHANKAR GHOSH, VINOTHAN MANOHARAN, Harvard University — We investigate the dynamics of placing individual colloidal particles (~2 microns) onto a flat oil-water interface using optical tweezers. By monitoring the position and strength of the trap, we are able to measure the forces acting on a particle as it encounters the liquid-liquid interface. Digital holographic microscopy affords us three dimensional position information at high frame rates (> 500fps), allowing us to probe short timescale behavior. We vary parameters such as particle surface chemistry, dissolved ion concentration, and pH in order to pursue questions about the nature of interface penetration dynamics.

5:06 PM L14.00014 Controlled Crystal Growth and Solid-Liquid Interface in temperature-sensitive colloidal systems. DUC NGUYEN, University of Amsterdam, The Netherlands, ZHIBING HU, University of North Texas, PETER SCHALL, University of Amsterdam, The Netherlands — We use temperature-sensitive colloidal NIPA systems to study crystal growth at the "atomic scale". By applying a temperature gradient we are able to control the growth of large colloidal single crystals. We visualize the nucleation of these crystals and solidification at the crystal-liquid interface in three dimensions by using confocal microscopy. Trajectories of particles on both the crystal and liquid side of an advancing interface are determined. These elucidate the mechanism of particle assembly at the interface of a growing crystal. At later stages of crystal growth, the interface becomes stationary, and we use the fluctuations of the stationary interface to determine the interface stiffness. Our data suggests a strong anisotropy of the interface tension. These microscopic observations provide unique insight into the mechanism of solidification.

5:18 PM L14.00015 A Surface Plasmon Resonance Investigation of How Water Meets a Hydrophobic Surface. ADELE POYNONOR, Allegheny College, Physics Department, COREY SHEMELYA — By definition hydrophobic substances hate water. Water placed on a hydrophobic surface will form a drop in order to minimize its contact area. What happens when water is forced into contact with a hydrophobic colloids surface? On the surface of a hydrophobic colloidal solution we have employed the surface-sensitive, quantitative optical technique of Surface Plasmon Resonance (SPR) to verify the existence of this region at the boundary.
1. **Single (non-fractal) characteristic cell size, but a scaling behavior of lengths and misorientations with external strain as the cellular structure refines. By adding deformation of crystals usually leads to the formation of cellular dislocation structures. Some experiments show fractal distributions of cell sizes; others show a density theory.**

2. **At low temperatures, climb-free plastic, YONG CHEN, WOOSONG CHOI, STEFANOS PAPANIKOLAOU, JAMES P. SETHNA, Laboratory of Atomic and Solid State Physics,**

3. **Cornell University, SURACHATE LIMKUMNERD, Physics Department, Chulalongkorn University, Bankok, Thailand — At low temperatures, climb-free plastic,**

4. **RG space. At late stages of the RG, there is a universal approach to the fixed point regardless of the initial distributions of frequency and coupling.**

5. **Although the RG was originally intended for strong randomness (distributions with long tails), we find good agreement with of phase-coupled oscillators in the regime of weak randomness. The RG predicts how oscillators with randomly distributed frequencies and couplings form frequency-synchronized clusters.**

6. **Control and Dynamical Systems, California Institute of Technology — We apply a recently developed renormalization group method to a 1-dimensional chain,**

7. **of phase-coupled oscillators in the regime of weak randomness. The RG predicts how oscillators with randomly distributed frequencies and couplings form frequency-synchronized clusters.**

8. **Although the RG was originally intended for strong randomness (distributions with long tails), we find good agreement with of phase-coupled oscillators in the regime of weak randomness. The RG predicts how oscillators with randomly distributed frequencies and couplings form frequency-synchronized clusters.**

9. **Control and Dynamical Systems, California Institute of Technology — We apply a recently developed renormalization group method to a 1-dimensional chain,**

10. **of phase-coupled oscillators in the regime of weak randomness. The RG predicts how oscillators with randomly distributed frequencies and couplings form frequency-synchronized clusters.**

11. **Control and Dynamical Systems, California Institute of Technology — We apply a recently developed renormalization group method to a 1-dimensional chain,**

12. **of phase-coupled oscillators in the regime of weak randomness. The RG predicts how oscillators with randomly distributed frequencies and couplings form frequency-synchronized clusters.**

3:06PM L15.00004 **ABSTRACT WITHDRAWN** —

3:18PM L15.00005 **Fixed point of a renormalization group approach for oscillator synchronization.**

3:30PM L15.00006 **Cell refinement and growing misorientations from a continuum dislocation density theory.**

3:42PM L15.00007 **Dynamic self-assembly in far-from-equilibrium magnetic granular ensembles at the liquid/liquid interface.**

3:54PM L15.00008 **Investigation on dynamics of colloidal particles with optically-controlled electrode patterns.**

4:06PM L15.00009 **Memories in paste: their applications to control crack patterns.**

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1. **This work was supported by the Korea Research Foundation (2006-1-D00058).**

2. **1** References [1] are omitted for brevity. For complete citation, please refer to the bibliography at the end of the document.
4:18PM L15.00010 Controlling chemical oscillations in heterogeneous BZ gels via mechanical strain. VICTOR YASHIN, Chemical Engineering Department, University of Pittsburgh; KRYSYTN J. VAN VLIET, Department of Materials Science and Engineering, Massachusetts Institute of Technology; ANNA C. BALAZS, Chemical Engineering Department, University of Pittsburgh — We performed theoretical and computational studies to determine the effect of an applied mechanical strain on the dynamic behavior of heterogeneous polymer gels undergoing the oscillatory Belousov-Zhabotinsky (BZ) reaction. In these gels, the catalyst for the reaction is localized in specific patches within the polymer network and the BZ reaction only occurs within these BZ patches. We focused on a 1D model for the system, and considered two scenarios, in which the BZ reaction did or did not affect the degree of swelling within the gel. For gels having one and two BZ patches, we found that a longitudinal strain could induce transitions between the oscillatory and steady state regimes. For certain values of the BZ stoichiometric parameter $f$, these transitions could exhibit a hysteresis. In systems having two oscillating BZ patches, a strain could switch between the in-phase and out-of-phase synchronization of the oscillations. The ability to alter the dynamic behavior of BZ gels through mechanical deformations opens up the possibility of using these materials in novel chemo-mechanical sensors.

4:30PM L15.00011 Rectification, Gating Voltage and Interchannel Communication of Nanoslot Arrays Due to Asymmetric Entrance Space Charge Polarization. GILAD YOSSIFON, YU-CHEN CHANG, HSUEH-CHIA CHANG, University of Notre Dame — A nanochannel array with homogenous surface charge height (i.e. uniform electro-chemical potential) but with asymmetric channel separation at the entrances is shown to exhibit strong rectification and gating type I-V characteristics at large voltage. Unlike previous low-voltage Ohmic studies of ionic current rectification within nano-pores/channels, which is attributed to intrinsic non-uniformity of the electro-chemical potential along the channel, this nanochannel array is due to asymmetric space-charge polarization and inter-channel communication at the entrances. This entrance polarization that controls the current flux at high voltages can overlap across nanochannels to render the array current very distinct from the collective current across isolated channels.

Wednesday, March 18, 2009 8:00AM - 11:00AM — Session P5 DFD DCOMP: Fluid Dynamics and Computational Science 401/402

8:00AM P5.00001 Inertial Particles in Turbulent Flows and the Clustering Instability of Interstellar Dust. PAOLO PADOAN, University of California, San Diego — The dynamics of dust grains in turbulent flows plays an important role in many astrophysical processes. I will review the problem of the formation of planetesimals (precursors of full-fledged planets) in turbulent circumstellar disks. I will then discuss some fundamental aspects of the physics of heavy particles in turbulent flows, and specifically the phenomenon of small scale clustering, an effect verified by laboratory experiments and in situ terrestrial cloud sampling. I will present results of large numerical simulations of particle-laden compressible turbulence, including statistics of clustering and of particle velocity differences.

8:36AM P5.00002 Multiscale modeling of the human arterial tree on the TeraGrid. GERORGE KARNIADAKIS, Brown University — A multiscale model of the human arterial tree will be presented consisting of the macrovascular network (MaN, arteries above 1-2 mm), the mesosvascular network (MeN, arterioles above 10 micro-m) and the microvascular network (MiN, capillaries). Coupling conditions between the MaN-MeN-MiN will be discussed and three different methods in modeling each network will be presented. Specific examples will be shown for the intracranial arterial tree for healthy subjects but also for patients with hydrocephalus.

9:12AM P5.00003 Terascale Direct Numerical Simulations of Turbulent Combustion. JACQUELINE CHEN, Sandia National Laboratories — The rapid growth in computational power in the past decade has presented both opportunities and challenges for high-fidelity simulations of turbulent reacting flows. The advent of terascale computing power has made it possible to glean fundamental physical insight into fine-grained “turbulence-chemistry” interactions in simple laboratory-scale turbulent flames from direct numerical simulation at moderate Reynolds numbers with detailed chemistry. Recent DNS results are presented to elucidate the role of autoignition and large-eddy mixing on the stabilization of a lifted ethylene-air jet flame in a heated coflow. The role of scalar dissipation rate on modulating ignition delays or lift-off heights is discussed. The simulations were performed at a jet Reynolds number of 10,000 and required 1.3 billion grid points to resolve the turbulence and flame structure. In a second related topic, the morphology of the scalar dissipation rate field in a turbulent jet flame is examined using topological methods, in particular the Morse-Smale Complex, which provides a natural segmentation of dissipation rate elements or “features.” These features are tracked in time, and conditional feature statistics are presented.

9:48AM P5.00004 Prediction and predictability of hurricanes with high-performance computers and cloud-resolving ensembles. FUQING ZHANG, Penn State University — This talk will be primarily devoted to the use of high-performance computing facilities to perform ensemble-based state estimation of hurricanes with cloud-resolving numerical weather prediction models. I will be sharing our recent experience in using approximately 30,000 cluster cores simultaneously at the Texas Advanced Computing Center which successfully assimilates high-resolution airborne Doppler radar observations in real time and subsequently delivers 2 deterministic and 60-member ensemble forecasts running at 4.5/1.5-km effective horizontal grid spacings in a timely fashion. Since the predictability of hurricanes may be fundamentally limited by chaotic moist convection and subsequent upscale error growth, I would advocate that besides the need of continuously improving the hurricane forecast models and ingesting high-resolution observations into the models to better initialize the storm, the hurricane state estimation is fundamentally probabilistic that demands cloud-solving ensemble-based data assimilation and forecasting. Improvements of forecast models may come from ever increasing computer power to better resolve the storms numerically and from improved fundamental understanding of the dynamics and impact of subgrid-scale turbulence in hurricanes. Improvements of better state estimation may also come from development of new theories that are applicable for high-dimensional, non-linear, non-Gaussian dynamic systems such as in hurricanes.

1Supported by the Division of Chemical Sciences, Geosciences, and Biosciences, Office of Basic Energy Sciences and the Office of Advanced Scientific Computing Research of the Department of Energy.

10:24AM P5.00005 On the two-way interactions between dispersed particles and turbulent flows. SAID ELOHOBASHI, Mech. and Aerospace Engineering Department, University of California, Irvine — Particle-laden turbulent flows are ubiquitous in nature (e.g. dust storms on Earth and Mars) and in industrial applications (e.g. liquid fuel and pulverized coal sprays in combustion chambers). Experimental and numerical studies of these flows are quite challenging due to the wide spectra of length- and time-scales of the dispersed particles in addition to the spectra of scales intrinsic to the carrier fluid turbulence. The two-way nonlinear interactions between the dispersed particles and the turbulence result in complex multi-scale physical phenomena. The lecture focuses on the physical mechanisms of the two-way interactions between dispersed spherical particles and simple turbulent flows using Direct Numerical Simulation (DNS). Particles whose diameter is smaller than the Kolmogorov length scale of turbulence are simulated as point particles. Results of particle-laden isotropic and homogeneous shear turbulent flows are presented. Particles with diameter larger than the Kolmogorov length scale are fully resolved using the Immersed Boundary method. Results of fully resolved particle-laden isotropic turbulence are presented.
8:00AM P14.00001 Measurement of the Force Network in a Dense Emulsion under Shear, S. K. DUTTA, E. KNOWLTON, D. L. BLAIR, Department of Physics, Georgetown University — We have investigated the properties of a dense oil-in-water emulsion under shear stress. Measurements of the jammed emulsion were taken with a customized confocal rheometer, which is capable of acquiring three-dimensional images while simultaneously applying a precise shear. Images acquired deep inside the emulsion are detailed enough to determine the position and shape of individual emulsion droplets. The forces on each droplet were calculated from the deformation due to neighbors, making it possible to link the bulk rheological properties of the emulsion to local structural relaxation and the force distribution measured at the single droplet level.

8:12AM P14.00002 ABSTRACT WITHDRAWN —

8:24AM P14.00003 Flow-Induced Droplet Deformation and Unjamming in Concentrated Emulsions under Large-Amplitude Oscillatory Shear, JUNG-REN HUANG, THOMAS G. MASON, University of California-Los Angeles — We employ the technique of shear oscillation light scattering to study concentrated oil-in-water emulsions subjected to oscillatory shear that causes droplet deformation and restructuring. Three dimensionless scattering intensity anisotropy factors, defined using the primary and secondary Bragg peak intensities, reflect the degree of droplet deformation caused by the applied shear. These factors distinguish the soft-jamming regime, where shear causes positional disorder, from the sliding hexagonally closed-packed layer regime, where shear induces positional order. Furthermore, near and above the jamming limit of spherical particles, the shear-induced droplet structure depends sensitively on the droplet volume fraction and the shear history.

8:36AM P14.00004 Structure and Rheology of Stimuli-Responsive Pickering Emulsions, DAN HO, PRASAD SARANGAPANI, YINGXI ELAINE ZHU, University of Notre Dame, Department of Chemical and Biomolecular Engineering, Notre Dame, IN 46556 — Self-assembly of micro- and nano-spheres and their stability at liquid-liquid interfaces are important due to their broad range of applications from emulsion polymerization to heavy oil transportation. In this work, we employ temperature-responsive poly(N-isopropyl acrylamide) (PNIPAM) microspheres to form Pickering emulsions and directly visualize the dynamics and rheology at the droplet interfaces in response to varied temperature using confocal laser scanning microscopy. Destabilization of the interface is observed as increasing temperature across the lower critical solution temperature (LCST) around 42-44 degree C for this system, where the coarsening at the oil-water interface occurs due to the shrinkage of PNIPAM particle size and results in the onset of coalescence of droplets.

8:48AM P14.00005 Shear Induced Dynamics of Polydisperse Jammed Emulsion Systems, JOAQUIM CLARA RAHOLA, ERIC R. WEEKS, Department of Physics, Emory University, Atlanta, GA, 30322 — We study polydisperse decane-in-water emulsions at droplet volume fractions ranging from $\phi = 0.65$ to $\phi = 0.9$. At such concentrations emulsions are jammed and thus droplet rearrangements are limited. To induce droplet displacements, an oscillatory strain is applied. We use confocal microscopy to track the trajectories of the droplets in real time and space. Almost all the droplets move periodically, but due to the polydispersity many of them move non-affinely as they are pushed around by other droplets. In these glassy suspensions, the motions of nearby droplets are correlated within a characteristic distance. This length is independent of particle volume fraction while it exhibits an increasing trend with increasing strain amplitude. Moreover, despite the disordered structure of our system, droplets’ motions are correlated over longer ranges than the average particle diameter.

9:00AM P14.00006 Colloidal Hydrodynamics with Arbitrary Boundary Conditions, JONATHAN K. WHITMER, ERIK LUIJTEN, University of Illinois at Urbana-Champaign — Hydrodynamic interactions are essential to the understanding of colloidal dynamics. Due to their complexity and computational cost, they are often ignored in simulations. Over the past decade, coarse-grained methods such as Stochastic Rotation Dynamics have been developed to include these interactions efficiently in simulation. To use these methods for the study of self-assembly dynamics of particles with anisotropic surface chemistry, we extend previously implemented methods for stick boundary conditions to arbitrarily slipping surfaces on the curved surfaces of spherical colloids. We present a mapping from a easily tunable simulation parameter onto the slip length as defined by Navier, and discuss the dynamics of anisotropic particles simulated using this method.

9:12AM P14.00007 Reversible Rayleigh-to-Mie Scattering Transition in a Core-Shell Colloidal System, GUANGNAN MENG, Harvard University, ADELINE PERRO, VINOTHAN MANOHARAN — We present a study of light scattering from colloidal particles with small polystyrene cores and large shells of poly(N-isopropylacrylamide-co-acrylic acid). When swollen by deionized water at room temperature, the shell is nearly index-matched to pure water, and the scattering is dominated by Rayleigh scattering from the polystyrene cores. As we change the solvent condition by increasing temperature or salt concentration, the shell starts to shrink and scatter light. Both the scattering cross section and the forward scattering of the particles increase, characteristic of Mie scatterers. We use optical microscopy, static light scattering and turbidimetry to study this optical transition. Such core-shell particles might be used as aqueous index-matched tracer colloids, as model scatterers for self-assembly studies, or as optical filters with tunable opacity.

9:24AM P14.00008 Pressure driven foam flow rheology, C. D. JONES, K. NORDSTROM, D. J. DURIAN, University of Pennsylvania — We probe the complex rheology of 3d foams by flowing them through a narrow column. The foam flows upward through one of two vertical rectangular columns with a 4.1 cross-sectional aspect ratio, by bubbling gas through a soapy solution at the base of our apparatus. One column is clear acrylic sheet on all sides, which is slippery to the foam, and results in plug flow. The other column has the narrow surfaces covered with sandpaper, giving them a sticky surface, which creates shear due to the zero velocity boundary condition. As expected, the flow profile between the slippery broad faces is flat, however the profile between the narrow, sticky faces exhibits a curved velocity profile that is strongly dependent on flow rate. We are able to analyze a 2d velocity profile from a 3d bulk system, whereas other recent foam rheology work has been constrained to the 2d system. We employ particle image velocimetry to measure the strain rate, and compute the stress from the pressure drop along the channel, to investigate the local stress-strain relationships in a flowing foam.
9:36AM P14.00009 Effective temperature of a sheared foam

DANIEL VALDEZ-BALDERAS, University of Rochester, PETER OLSSON, Umea University, STEPHEN TEITEL, University of Rochester — We perform computer simulations of a model for an overdamped, sheared foam in two dimensions at zero temperature. We measure an effective temperature with the use of an embedded oscillator, in manner analogous to experiments done by Abate and Durian on a different system [arXiv:0806.0765v2]. Our oscillator is one of the bubbles in the foam, which, in addition to its interaction with other bubbles, is also subject to a harmonic potential. We define an effective temperature based on the fluctuations in the position of the oscillator. We compare our results to the effective temperatures computed with the use of measurements of the fluctuations of the shear stress and fluctuations of the energy, respectively.

1Supported by DOE Office of Basic Energy Sciences, grant DE-FG02-06ER46298

9:48AM P14.00010 Realization spaces of bubble clusters and coarsening trajectories

RANDALL KAMEN, University of Pennsylvania — In the search for a more unified description of the geometry of equilibrium foams, we study the space of all realizations of equilibrium bubble clusters of fixed topology. The geometry of foam is highly constrained due to the area minimization property - in two dimensions, this means that all interfaces must be portions of circles and interfaces intersect in threes at angles of 120°. This results in a finite dimensional space of bubble clusters, and the dynamics of coarsening via gas diffusion induces a vector flow on it. The boundaries and singularities of the realization space may be identified with topological transitions and instabilities in coarsening.

10:00AM P14.00011 Experimental studies of low-density fluid phases in tunable dipolar colloids

ANAND YETHIRAJ, NING LI2, HUGH NEWMAN, MANUEL VALERA3, IVAN SAIKA-VOIVOD, Memorial University — Experiments of low-density colloidal fluid phases in the presence of an external electric field are presented. We obtain angular order parameters as a function of the applied electric field. When plotted against a dimensionless dipolar strength parameter, the order parameters for different particle sizes fall on a single curve, suggesting that colloids in a fluid phase in the presence of electric fields do indeed interact by an effective point dipolar interaction. We then explore the statistics of particle packings at low-density and extract the experimental compressibilities and equation of state for these dipolar colloids.

1This work is being supported by NSERC
2(present address: Brandeis University)
3(present address: Slippery Rock University)

Wednesday, March 18, 2009 8:00AM - 11:00AM
Session P15 DFD: Biologically Inspired Physics: Swimming, Propulsion, Bio-fluids

8:00AM P15.00001 Swimming in a vortex street

SILAS ALBEN, Georgia Tech — Recent studies showed that a trout swimming in a cylinder wake can save energy by “salomeling” through a vortex street. We present a simple model using a flexible body with vortex sheets, and find swimming shapes which maximize output power and efficiency. We find analytic solutions and compare the optimal swimming phase between the body and vortices with previous experiments and numerics.

1NSF-DMS support is acknowledged.
8:48 AM P15.00005 Accumulation of microswimmers near surface due to steric confinement and rotational Brownian motion, GUANGLAI LI, JAY TANG, Brown University — Microscopic swimmers display some intriguing features dictated by Brownian motion, low Reynolds number fluid mechanics, and boundary confinement. We re-examine the reported accumulation of swimming bacteria or bull spermatozoa near the boundaries of a fluid chamber, and propose a kinematic model to explain how collision with surface, confinement and rotational Brownian motion give rise to the accumulation of micro-swimmers near a surface. In this model, an elongated microswimmer invariably travels parallel to the surface after hitting it from any incident angle. It then takes off and swims away from the surface after some time due to rotational Brownian motion. Based on this analysis, we obtain through computer simulation steady state density distributions that reproduce the ones measured for the small bacteria E coli and Caulobacter crescentus, as well as for the much larger bull spermatozoa swimming near surfaces. These results suggest strongly that Brownian dynamics and surface confinement are the dominant factors for the accumulation of microswimmers near a surface.

9:00 AM P15.00006 Modeling the Behavior of Self-Propelled Microcapsules, AMITABH BHATTACHARYA, Dept of Chemical Engg, University of Pittsburgh, O. BERK USTA, ANNA C. BALAZS, Dept of Chemical Engg, Univ Pittsburgh — Biological cells can perform complex tasks by signaling and moving autonomously in their environment. We study a system of self-propelled microcapsules, first proposed by Usta et al (2008), that mimics this process. It consists of a signaling and target microcapsule placed close to an adhesive substrate and immersed in fluid. The signaling microcapsule encases nanoparticles, which, when released, modifies the adhesive strength of the substrate. The adhesion gradients in the substrate, along with hydrodynamic interactions among the capsules, gives rise to a sustained motion of the microcapsules. In this work, we perform simulations (based on lattice Boltzmann method for the fluid and random walk simulation for nanoparticles) of several signal-target configurations, consisting of two or more rigid capsules. In particular, we examine a configuration consisting of a single signaling capsule pushing multiple target capsules in a single file. For a constant release rate of nanoparticles, the velocity of the train of capsules asymptotes to a constant value at large times. Using a low-order analytical model for this system, we show that there is a simple relationship between this asymptotic velocity and the parameters in the system (e.g. number of capsules, release rate of nanoparticles, viscosity of fluid, adhesive strength of substrate etc.).

9:12 AM P15.00007 Mixing fluid by self-propelled objects, MAXIM BELKIN, Illinois Institute of Technology / Argonne National Lab, ALEXEY SNEZHKO, IGOR ARANSON, WAI-KWONG KWOK, Argonne National Lab — Magnetic microparticles suspended at the water-air interface and subjected to an ac external driving self-assemble into dynamic structures (magnetic snakes). The snakes are accompanied by four large hydrodynamic vortices. At high enough frequencies and amplitudes of driving the snakes transform into self-propelled swimmers. Moving erratically, these swimmers mix the surface of fluid at a very high rate. We performed detailed experimental studies of these self-organized mixing. We studied space and time correlation and diffusion process in such systems.

9:24 AM P15.00008 Enskog-theory for stochastic models with self-propelled and passive particles, ALEMAYEHU GEBREMIARAM, THOMAS IHLE, Department of Physics, North Dakota State University — Macroscopic evolution equations for interacting many-body systems do not just ‘emerge’; they follow from microscopic laws. However, it is often difficult to quantitatively establish this link, especially for systems which cannot be described by a Hamiltonian and which do not have pairwise additive interactions. Therefore, the general form of the macroscopic equations is usually obtained by symmetry arguments. Here, using a particle-based model with discrete time evolution steps for fluid flow I show how the macroscopic transport equations can be rigorously derived from microscopic collision rules. The approach starts with the full N-particle Liouville equation and leads to a multi-particle Enskog-equation which is treated by a Chapman-Enskog expansion. No linearization or single-relaxation time approximation of the collision operator is needed. The obtained thermo-hydrodynamic equations show excellent agreement with previous numerical results. The same approach is used to study a simple model of self-propelled, swarming birds. This model was proposed by T. Vicsek et al. [Phys. Rev. Lett. 75 (1995) 1226]; it has ‘multi-particle collisions’ where birds within some interaction range align their flying directions. I analytically analyze the collision-operator for small and large bird density, and derive the hydrodynamic equations for the density and velocity fields.

9:36 AM P15.00009 The “caterpillar” simulation model for a biological filament, AIMEE BAILEY, Imperial College London, CHRISTOPHER LOWE, Universiteit van Amsterdam, ADRIAN SUTTON, Imperial College London — We present a simulation model for an elastic filament in a viscous fluid, relevant for systems ranging from suspensions of paper pulp to micro-organism motility. It incorporates the Stokeslet treatment of the hydrodynamic force. We show that a non-ordinary choice of the hydrodynamic radius is necessary to recover known dynamic behavior of a fiber with a finite cross-section. Our simulations explore configurations inaccessible by theory. We illustrate the utility of the model by considering the simple scenario of a charged filament in an electric field. Results suggest a circularly polarized electric field is a viable means for aligning microtubules in solution.

9:48 AM P15.00010 Flow and nutrient transport through porous scaffolds used for the culture of bone cells in perfusion bioreactors, DIMITRIOS PAPAVASSILIOU, The University of Oklahoma, ROMAN VORONOV, VASSILIOS SIKAVITAS, The University of Oklahoma, SAMUEL VANGORDON — The goal is to understand via computation the behavior of the flow inside porous scaffolds that are used in bone tissue bioreactors. Fluid shear is an important stimulatory factor in preosteoblastic cells seeded in scaffolds and cultured under continuous flow perfusion. A Lattice Boltzmann method has been employed to simulate the flow field within porous scaffolds obtained with high resolution micro-CT. Lagrangian methods have also been used to determine the nutrient dispersion inside the scaffolds. The shear stresses calculated inside the scaffold architecture indicate that the shear stresses experienced by cells inside the scaffold can vary by orders of magnitude. This is important when designing scaffolds for bone tissue growth, since osteoblastic cells require to be stimulated by shear for growth. Moreover, cell detachment can occur when the fluid shear is too high, thus, placing a limit on the stresses that a particular scaffold design should allow. The talk will address the methodology, the validation and the correlation of scaffold structure characteristics with the shear stresses and with the rate of mass transfer.

10:00 AM P15.00011 Instabilities and waves in thin films of living fluids, SUMITHRA SANKARARAMAN, SRIRAM RAMASWAMY — We formulate the thin-film hydrodynamics of a suspension of polar self-driven particles and show that it is prone to several instabilities through the interplay of activity, polarity and the existence of a free surface. Our approach extends, to self-propelling systems, the work of Ben Amar and Cummings [Phys Fluids 13 (2001) 1160] on thin-film nematics. Based on our estimates the instabilities should be seen in bacterial suspensions and the lamellipodium, and are potentially relevant to the morphology of biofilms. We suggest several experimental tests of our theory.
10:12AM P15.00012 Tuning inter-virus interactions in natural aquatic environments. NATHAN W. SCHMIDT, Department of Physics, University of Illinois, Urbana-Champaign, ANDREW K. UDIT, Department of Chemistry, Scripps Research Institute, LEONARDO GUTIERREZ, THANH H. (HELEN) NGUYEN, Civil and Bioengineering, University of Illinois, Urbana-Champaign, M.G. FINN, Department of Chemistry, Scripps Research Institute, GERARD C.L. WONG, Department of Materials Science and Engineering, University of Illinois, Urbana-Champaign — Polymeric natural organic matter (NOM) originating from plants and animals is ubiquitous in natural aquatic environments. Many water-borne pathogens, including viruses, readily associate with NOM, which has a statistical distribution of charged and hydrophobic groups. Virus-NOM association influences the transport of viruses in groundwater environments, but little is known about this interaction, or how NOM can induce new inter-virus interactions. To better understand the interaction between NOM and aqueous contaminants, we use the MS2 and Qbeta viruses (diameters ∼ 27nm) as surrogate water-borne pathogens. Small Angle X-ray Scattering is used to characterize the inter-particle interaction between viruses over a range of NOM concentrations and different salt types and concentrations.

10:24AM P15.00013 Computational studies on characteristic fluid behavior in the stented cerebral aneurysm. MIHI HIRABAYASHI, University of Geneva, MAKOTO OHTA, DANIEL A. RÜFENACHT, Hospital University of Geneva, BASTIEN CHOPARD, University of Geneva — We present a computational analysis of the fluid behavior in the stented aneurysm. It is important to reveal the complex mechanism of the velocity reduction of the flow in the stented aneurysm in order to design the effective stent, which is a tubular mesh of wires placed for the treatment of the cerebral aneurysm. To understand the effect of a stent we already proposed a quantitative analysis of the flow pattern in the stented aneurysm. Here we present a quantitative analysis of the transition of the pressure and the shear stress caused by the changes of the flow pattern to verify the velocity reduction mechanism of the stent. We expect that our study will lead to a new suggestion for the effective treatment of the cerebral aneurysm by the stent.

10:36AM P15.00014 Run length is the dimension that characterizes path integrals useful for designing passive bacterial pumps1. DAVID LIAO, GUILLAUME LAMBERT, Department of Physics, Princeton University, Princeton, NJ 08544, PETER GALAJDA, Delft University of Technology, CJ Delft, The Netherlands, ROBERT AUSTIN, Department of Physics, Princeton University, Princeton, NJ 08544 — Asymmetric funnels have been used as passive pumps to concentrate Escherichia coli in nanostructured devices (Austin 2007). Funnel geometry changes pump efficiency, which could be important when driving cell sorters (Whitesides 2008). The larger set of funnel geometries that could be considered when designing pumps motivated us to derive a path-integral-like formula to predict the flux produced by arbitrary funnel geometries. We applied this equation to a two-dimensional wedge-shaped funnel. Model and experiment agree that the steady-state ratio between concentrations on two sides of a funnel open to 60◦ is 3 when the aperture is one fifth the bacterial run length and 1 when the aperture is 16 times the run length, an example of how the run length here has a role loosely analogous to the wavelength in quantum mechanical path integrals.

10:48AM P15.00015 Selective transport through nano-channels: do we understand it? ANTON ZILMAN, Los Alamos National Laboratory, T. JOVANOVIC-TALISMAN, B. CHAIT, M. ROUT, S. DI TALIA, M. MAGNASCO, Rockefeller University — Functioning of living cells requires selective molecular transport, which is provided by transport channels that are able to selectively transport certain molecular species while filtering others, even similar ones. Such channels can selectively transport their specific molecules in the presence of vast amounts of non-specific competitors. In many cases, efficient and selective transport occurs without direct input of metabolic energy and without transitions from an ‘open’ to a ‘closed’ state during the transport event. Examples include selective permeability of porins and transport through the nuclear pore complex. Mechanisms of selectivity of such channels have inspired design of artificial selective nano-channels, which mimic the function of selective biological channels. Mechanisms of selectivity of such nano-channels are still unknown. I present a theoretical model to explain the selectivity of transport through nano-channels, which contains only the essentials of stochastic kinetics inside the channel. The theory provides a mechanism for selectivity based on the differences in the kinetics of transport through the channel between different molecules. The theory explains how the specific molecules are able to filter out the non-specific competitors - and proposes a mechanism for sharp molecular discrimination. The theoretical predictions account for previous experimental results and have been verified in ongoing experiments.

Wednesday, March 18, 2009 11:15AM - 1:51PM – Session Q14 DFD: Granular Fluctuations 315

11:15AM Q14.00001 Cooling and aggregation in wet granulates. ANNETTE ZIPPELNIUS, STEPHAN ULRICH, TIMO ASPELMIEIER, University of Goettingen, KLAUS ROELLER, AXEL FINGERLE, STEPHAN HERMINGHAUS, Max-Planck-Institute for Dynamics and Self-Organization. Wet granular materials are characterized by a defined bond energy in their particle interaction such that breaking a bond implies an irreversible loss of a fixed amount of energy. Associated with the bond energy is a nonequilibrium transition, setting in as the granular temperature falls below a certain threshold. The subsequent aggregration of particles into clusters is shown to be a self-similar growth process with a cluster size distribution that obeys critical scaling. In the early phase of aggregation the clusters are fractals with Df = 2, for later times we observe gelation. We use simple scaling arguments to derive the temperature decay in the early and late stages of cooling and verify our results with event-driven simulations.

11:27AM Q14.00002 Propagating Waves in a Monolayer of Self-Propelling Gas-Fluidized Rods. LYNN J. DANIELS, DOUGLAS J. DURIAN, University of Pennsylvania — We report on the existence of propagating compression waves in a quasi-two-dimensional monolayer of self-propelling rods fluidized by an upflow of air. This behavior is unique to rods; a comparable system of spheres exhibits no waves and displays ‘thermal’ number fluctuations, proportional to N^{1/2}. The waves, however, give rise to anomalously large number fluctuations, having both magnitude and exponent greater than ‘thermal’ fluctuations. This occurs as rarefaction zones relax after a compression front has traveled through a region. We characterize the waves by calculating a dynamic structure factor. The position of observed peaks, as a function of frequency ω and wavevector k, yield a linear dispersion relationship in the long-time, long-wavelength limit and a wavespeed ω/k = 20 cm/s. By contrast, spheres exhibit 1/ω^2 decay for all wavevectors in the hydrodynamic limit, consistent with the diffusive decay of density fluctuations.
11:39AM Q14.00003 Phase diagram of wet granular matter under vertical vibrations, KAI HUANG, KLAUS ROELLER, STEPHAN HERMINGHAUS, Max Planck Institute for Dynamics and Self-organization — The phase diagram of vertically vibrated wet granular matter is investigated by both experiments and simulations. We find a critical point where the coexistence (C) regime of the fluid (F) and gas (G) phases terminates. The energy driven F-C transition is found to scale with the rupture energy of a liquid bridge if the corresponding vibration amplitude A is less than particle diameter d. This is in good agreement with our simulations. Close to the F-G transition line, the variation of the size of the gas bubble with vibration amplitude shows a hysteretic behavior. Within the hysteresis loop, we observe temporary gas bubbles with strong fluctuations in size. The F-G boundary is present above an interfacial tension in non-trivial wetting behavior at container walls. Focusing on the solid (S)-F transition line, we find that the fluidization is a surface melting process. This is demonstrated by detecting the mobility of ruby tracers utilizing ruby fluorescence. This as well agrees with our simulation results.

11:51AM Q14.00004 Stress wave mitigation in granular media, CHIARA DARIAO, CALTECH, F. FERNANDO, University of Salerno, Italy, MASON PORTER, Oxford University, UK — We study stress wave mitigation in one- and two-dimensional granular media employing evolutionary algorithms to investigate the optimal design of composite protectors using granular chains composed of beads of various sizes, masses, and stiffnesses. We define a fitness function using the maximum force transmitted from the protector to a wall that represents the body to be protected and according to the setup we propose, we optimize the protector design. The optimization is carried out using the Discrete-Element Method and experiment (using glass beads, imaged via an index-matched fluid). We begin by performing a quantitative comparison between the two procedures, concentrating on the level of agreement at the microscopic scale. After establishing how well the simulation can reproduce the microscopic fluctuations in particle velocities seen in experiment, we proceed to carry out a tensile analysis of granular temperature. Our results show different exponents and prefactors of the dissipative terms in the equations of motion. We thus propose a quantitatively-accurate extension of the Hertzian model encompassing realistic material dissipative effects. Experiments and computations with steel, brass, and polytetrafluoroethylene reveal a common dissipation exponent (for a discrete Laplacian of the velocities) with a material-dependent prefactor.

12:03PM Q14.00005 Anisotropies in granular temperature in a dense sheared granular flow, CHRIS RYRCROFT, University of California, Berkeley and Lawrence Berkeley Laboratory, ASHISH ORPE, National Chemical Laboratory, India, ARSHAD KUDROLLI, Clark University — We investigate a three-dimensional, slow, gravity-driven, sheared granular flow, making use of both simulation (carried out using the Discrete-Element Method) and experiment (using glass beads, imaged via an index-matched fluid). We begin by performing a quantitative comparison between the two procedures, concentrating on the level of agreement at the microscopic scale. After establishing how well the simulation can reproduce the microscopic fluctuations in particle velocities seen in experiment, we proceed to carry out a tensile analysis of granular temperature. Our results show different types of behavior near the boundary and in the bulk of a granular flow, due to differences in the particle packing structure, and highlight anisotropies that may have implications for granular continuum modeling.

12:15PM Q14.00006 Correlation Functions of a Homogeneously Driven Granular Fluid in Steady State, KATHARINA VOLLMAYR-LEE, Bucknell University, TIMO ASPLEMEIER, ANNETTE ZIPPELIUS, Georg-August-Universität Goettingen, Germany — We study a homogeneously driven granular fluid of hard spheres at intermediate volume fractions and focus on time-delayed correlation functions in the stationary state. The results of computer simulations using an event-driven algorithm are compared to the predictions of generalized fluctuating hydrodynamics. The incoherent scattering function \( F_{\text{incoh}}(q, t) \) follows time-supercorrelation and is well approximated by a Gaussian \( F_{\text{incoh}} = \exp \left( -\frac{q^2}{2} \langle \Delta r^2(t) \rangle \right) \). For sufficiently small wavenumber \( q \) we observe sound waves in the intermediate scattering function \( F(q, t) \) and in the longitudinal current correlation function \( C_L(q, t) \). We determine their dispersion and damping. Temperature fluctuations are predicted to be either diffusive or nonhydrodynamic, depending on wavenumber and inelasticity as characterized by incomplete normal restitution.

12:27PM Q14.00007 Interparticle friction between gently contacting spheres, GREG FARRELL, NARAYANAN MENON, Dept of Physics, UMass Amherst — In previous experimental work we have found that the packing fraction of gently-sedimented monodisperse spheres is affected by particle roughness as well as the viscosity and buoyancy provided by the surrounding fluid. In order to provide a macroscopic quantification of the microscopic effects of particle surface and of the fluid, we have developed a new technique to measure the coefficients of static and kinetic friction between two spheres in a fluid. We find that even in fluid environments, there are static and kinetic coefficients of friction characteristic of solid-on-solid contact. Surprisingly, even for a given pair of spheres, we measure a broad range of friction coefficients corresponding to contacts made at different locations on the surface. Thus, even for lubricated surfaces, surface heterogeneity is more apparent for small normal forces than at familiar force-scales.

We acknowledge support through NSF-DMR 0606216.

12:39PM Q14.00008 Spatial Force Correlations in 3D Granular Flow, NALINI EASWAR, KELSEY HATTAM, EFROSYNI SEITARIDOU, ALISA STRATULAT, Smith College. Northampton, MA., NARAYANAN MENON, University of Massachusetts, Amherst, MA, — We measure the force delivered at four locations on the boundary of a 3D flow of mono-disperse glass spheres in a vertical, cylindrical chute. A variable opening at the bottom is used to change the flow velocity \( v_f \) from 3 to 30cm/s. The force is measured at 80KHz, allowing us to resolve individual collisions. We measure two-point spatial correlations in the flow direction and normal to it. The equal-time correlation between forces that are higher than a threshold shows a weak but measurable spatial correlation. This correlation shows no spatial directionality or dependence on flow rate. The time correlations are synchronous between diametrically opposed locations, and shifted in time between locations along the flow. From the time-lag we determine that the correlations are carried up the flow at speeds \( \sim 1000 v_f \). This speed increases as the flow approaches jamming.

Supported by NSF DMR 0606216 and NSF MRSEC DMR 0213695

12:51PM Q14.00009 Impact phenomena in fluidized granular matter, PATRICK MAYOR, HIROAKI KATSURAGI, DOUGLAS DURIAN, University of Pennsylvania, Philadelphia — Projectiles dropped into granular media form a crater and come to rest in a particular way that has been actively investigated in numerous studies. These impact phenomena illustrate how particulate materials respond to externally applied forces. Several recent experiments have focused on the penetration of projectiles impacting granular materials at relatively low speeds, and measured the dynamics of the impact process, yielding force laws accounting for the observations. We present results showing how granular impacts are affected when the load on the grains is modified using a vertical gas flow. Balls or cylinders are dropped into a dry, noncohesive granular medium and we measure the penetration depth when gas is flown upward (thus unloading the contacts) or downward (loading the contacts). We observe that the frictional drag decreases linearly with the flow rate, and vanishes completely once the system is fluidized. Different projectile geometries allow us to separate the effects of normal and tangential frictional forces. We also consider the case of objects that are lowered quasi-statically into the granular medium and measure the net vertical force exerted by the granular system on the objects at each immersion depth. We then discuss how this resistance force compares with the forces observed in actual impacts experiments.
We investigate the efficacy of a square-grid mesh at filtering rods from solution. The volume fraction \( \phi \) is kept low, reducing the chance of rods cooperatively jamming at the mesh. For round particles, filtering at low \( \phi \) is trivially determined by the ratio of particle diameter to mesh size. Because rods have two length scales, filtering is non-trivial for meshes larger than the rod width but smaller than the length, a potentially very large range. We have measured experimentally the probability for a rod to be filtered as a function of mesh size, particle length, and aspect ratio. Results are compared with a theoretical extension of the Buffon-Laplace Needle problem that accounts for finite rod width and an isotropic distribution in the zenith angle. The solution is the probability that a spherocylinder in three dimensions makes contact with a 2D sieve-like mesh, a necessary but not sufficient condition for filtration.

Results are compared with a theoretical extension of the Buffon-Laplace Needle problem that accounts for finite rod width and an isotropic distribution in the zenith angle. The solution is the probability that a spherocylinder in three dimensions makes contact with a 2D sieve-like mesh, a necessary but not sufficient condition for filtration.

The Free energy of the landscape is calculated using these tiles and we discuss the role of these tiles in the liquid to liquid transition. The complete jamming local jamming structures to construct globally jammed states. We discuss the role of these tiles in the thermodynamic behavior of the corresponding liquid.

Continuous driving results in the phenomenon of granular breathing. The talk shall discuss the dynamical processes associated with granular breathing for time-independent and time-dependent driving. The phenomenon of nonlinear resonant and related processes that arise in these systems will be discussed.

The Free energy of the landscape is calculated using these tiles and we discuss the role of these tiles in the liquid to liquid transition. The complete jamming local jamming structures to construct globally jammed states. We discuss the role of these tiles in the thermodynamic behavior of the corresponding liquid.

Supported in part by a grant from the National Science Foundation, Division of Materials Research.

We study the dynamics of monodispersed and tapered granular alignements held within a fixed boundary and a moving boundary. The system is assumed to be driven at one end by imparting a constant or time dependent acceleration to the edge grain. Analytical and simulational studies show that such a driven system can eventually get “over-compressed” and begin to dilate due to repulsive grain-grain interactions. Continuous driving results in the phenomenon of granular breathing.
3:06PM T14.00004 Hydrogen-bond network dynamics in sugar-based glasses, MARCUS CICERONE, JERAINNE JOHNSON, NIST, MICHAEL PIKAL, University of Connecticut — Hydrophilic organic glasses composed of sugars and polysaccharides are known to stabilize proteins against aggregation and chemical degradation. It has long been supposed that, due to the long timescales involved in protein aggregation and chemical degradation in the glass, β relaxation processes essentially control the rate of degradation. We have shown that, although there may be > 7 orders of magnitude in time separation, β relaxation processes can dominate in influencing both chemical and physical degradation. Also, it is apparent that these β processes are closely related to dynamics of the hydrogen-bond network in these glasses. In this presentation we will briefly discuss the phenomenology of protein degradation in sugar-based glasses, and also present details of work on developing a fluorescent probe for use as a sensor for dynamics of the hydrogen-bond network in these glasses.

3:18PM T14.00005 Density of states and soft modes of hard sphere colloidal glasses — experimental observations, ANTINA GHOSH, VIJAYAKUMAR CHIKKADI, PETER SCHALL, University of Amsterdam, The Netherlands, JORGE KURCHAN, ESPCI, France, DANIEL BONN, University of Amsterdam, The Netherlands — Recent theories and simulations have predicted the presence of soft modes due to which the DOS of glassy materials does not go to zero at zero frequency. We obtain DOS of colloidal hard sphere suspensions from experimental data. The displacement fields of hard sphere colloidal suspensions were studied for a range of volume fractions near the glass transition using confocal microscope. Normal mode frequencies are then computed from the time averaged correlation matrix. The density of vibrational states obtained from normal mode analysis indeed reveals an excess of low frequency anomalous modes in the system. To understand the nature of the modes we analyse the displacement vector fields at various frequencies.

3:30PM T14.00006 XPCS Studies of Nanoparticle Motion within Glassy Polymer Melts, H. GUO, JHU, G. BOURRET, R. B. LENNOX, M. SUTTON, McGill U., J. L. HARDON, U. of Ottawa, R. L. LEHENY, JHU — We report x-ray photon correlation spectroscopy (XPCS) experiments to investigate the motion of nanoscale gold particles within poly styrene (PS) melts of molecular weight between 2K and 48K g/mol. The particles, with radius of approximately 2 nm, are dispersed in a highly dilute concentration (volume fraction 0.0004) and are functionalized with PS chains to stabilize them against aggregation. At high temperature, the observed motion is diffusive, with a rate that follows a Vogel-Fulcher temperature dependence. When the melts are quenched to lower temperature, the XPCS results indicate hyper-diffusive motion that can be modeled as strain in the melt in response to localized stress relaxation. These dynamics evolve with time following the quench, suggesting that they are coupled to aging of the polymer. Our observation of this hyper-diffusive motion among such a dilute concentration of stable nanoparticles indicates that the particles act as passive tracers and the motion is an intrinsic property of quenched melts.

3:42PM T14.00007 Divergent four-point dynamic density correlation function of a glassy suspension, GRZEGORZ SZAMEL, ELIJAH FLENNER, Department of Chemistry, Colorado State University — We use a diagrammatic formulation of the dynamics of interacting Brownian particle${}^1$ to study a four-point dynamic density correlation function of a glassy colloidal suspension. We re-sum a class of diagrams which separate into two disconnected components upon cutting a single propagator. The resulting formula for the four-point correlation function can be expressed in terms of three-point functions closely related to the three-point susceptibility introduced by Biroli et al${}^2$ and the standard two-point correlation function. We numerically evaluate the four-point function and the associated dynamic correlation length. Both the amplitude of the four-point function and the correlation length diverge at the mode-coupling transition.

3:54PM T14.00008 Self-Organized Criticality in Periodically-Sheared Sedimenting Suspensions, EMMANOUELA FILIPPIDI, Center for Soft Matter Research, New York University, LAURENT CORTE, Centre des Matériaux Mines, Paris, France, PAUL CHAIGIN, Center for Soft Matter Research, New York University, LAURENCE RAMOS, Univerisite Montpellier II and CNRS, France, DAVID PINE, Center for Soft Matter Research, New York University — Suspensions of non-colloidal particles under slow periodic strain can undergo a dynamical phase transition from an active fluctuating state to an absorbing steady state at a critical volume fraction. In the case of density-mismatched particles, sedimentation and shear-induced diffusion drive the system towards a self-organized critical state. The length scales and timescales associated with the dynamics of the active particle clusters sustained near the critical point are shown to follow power-law behavior via simulation of activated random walkers. Finite-size effects and excluded volume interactions are explored for sedimenting and neutrally buoyant, mono- and bi-disperse suspensions both by simulation and experiment.

4:06PM T14.00009 Heat transfer in model amorphous solids, VINCENZO VITELLI, NING XU, Department of Physics, University of Pennsylvania, MATTHIEU WYART, HSEAS, Harvard University, ANDREA LIU, Department of Physics, University of Pennsylvania, SIDNEY NAGEL, James Frank Institute, University of Chicago — We investigate heat transfer in model amorphous solids obtained from jammed packings of soft spheres. At the boson peak frequency, we find a sharp crossover from a weak-scattering regime, in which the energy diffusivity drops rapidly with frequency, to a strong-scattering regime, in which the diffusivity is nearly frequency-independent. We present a scaling analysis of how the crossover frequency shifts to zero as the system is decompressed towards the jamming transition. We show that the regime of flat diffusivity, invoked to explain the temperature dependence of the thermal conductivity of glasses, can arise from properties of the jamming transition.

4:18PM T14.00010  Structural response of a colloidal glass to local forcing, KEVIN B. APTOWICZ, West Chester University, PETER J. YUNKER, University of Pennsylvania, SEAN GOSSIN, West Chester University, ZEXIN ZHANG, A. G. YODH, University of Pennsylvania — Video microscopy of glassy colloidal suspensions permits direct visualization of particle locations and trajectories, thereby providing an excellent experimental tool to aid our understanding of glasses and address current theories. We have conducted a set of experiments utilizing a bidisperse mixture of thermosensitive NIPA microgel spheres to study the structural response of a two-dimensional colloidal glass to point expansion. The packing fraction of the colloidal suspension is tuned from a liquid to a deeply jammed glass by varying the global temperature of the sample. Over this range of packing fractions, the response of the sample to point expansion is analyzed. In particular, an infrared laser tightly focused on the sample generates thermophoretic forces that lead to a point expansion in the colloidal glass. We track particle rearrangements and characterize the response as a function of packing fraction. These experiments take a step towards understanding the relationship between local structure and bulk properties of glass.

This research is supported by MRSEC grant DMR-0520020 (AGY), NSF grant DMR-080488 (AGY) and an award from Research Corporation (KBA).
4:30PM T14.00011 Relaxation processes in polystyrene melts and ultra-thin films, A. BALJON, S. WILLIAMS, San Diego State University, N. BALABAЕV, Institute of Mathematical Problems of Biology, Pushchina, Russia, F. PAANS, A. LYULIN, Dutch Polymer Institute, Technical University Eindhoven, The Netherlands — By means of large-scale computer simulations we investigate relaxation processes in polystyrene melts and ultra-thin films. The local orientational mobility of the phenyl bonds is studied with the help of Legendre polynomials of the second-order $P_2(t)$. The spectral density of $P_2(t)$ shows several distinctive peaks. They are caused by the large-scale motions of cooperative segments.

4:42PM T14.00012 Changes in Local Structure and Dynamic Heterogeneity in an Aging Glass, PETER YUNKER, ZEXIN ZHANG, University of Pennsylvania, KEVIN B. APTOWICZ, West Chester University, AHMED M. ALSAYED, CNRS/Rhodia, ARJUN YODH, University of Pennsylvania — Recent works have shown a connection between structure and dynamical heterogeneity in glass. However, a connection between structure and aging dynamics remains elusive. To this end, we study aging in a bidisperse suspension of soft spheres. Micron-sized temperature-sensitive NIPA particles are employed in two-dimensions, and directly observed with video microscopy. After quenching from liquid to glass, the fraction of particles with crystalline order within the first coordination shell increases with time. Particles that undergo irreversible rearrangements, the aspect of dynamic heterogeneity most closely linked to structural relaxation, are identified. Particles with local crystalline order are observed to be very unlikely to irreversibly rearrange, and therefore more stable. This increase in stable particle configurations leads to the slowing of dynamics that is characteristic of aging.

4:54PM T14.00013 Investigation of electron beam induced changes in glassy Ge$_x$Se$_{1-x}$ thin films, W. ZHOU, G. HOFFMAN, H.O. COLIN, R.M. REANO, S. SOORYAKUMAR, The Ohio State University, P. BOOLCHAND, University of Cincinnati — Global structures in network glasses are characterized by their connectedness or mean coordination number. As the number of these cross-links within a covalent network increases by compositional tuning these systems steadily evolve from being underconstrained (floppy) to an overconstrained (rigid) solid. Recently (Appl Phys Lett 93, 041107 (2008)) we exploited electron beams to write nanoscale surface motifs in Ge$_{0.2}$Se$_{0.8}$ thin films that are at the special Ge in Se composition lying in the immediate vicinity of the floppy to rigid stiffness transition. In order to investigate the nature of the surface reliefs we have employed selected area transmission electron microscopy (TEM) to probe the electron beam induced structural changes to the film. Films of thicknesses less than 150 nm were deposited by pulsed laser deposition directly onto a carbon film on a mica substrate. The glass film and carbon layer were then lifted off onto copper grids for the TEM studies. Extension of the electron beam driven studies to other compositions, as well as the effect of multiple beam overwrites on the surface reliefs and trenches in several Ge$_x$Se$_{1-x}$ compositions will also be presented.

5:06PM T14.00014 Periodic Lattices Near Isostaticity, ANTON SOUSLOV, T.C. LUBENSKY, Dept. of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104 — Lattices in $d$ dimensions with with an average of $z = 2d$ contacts per site are at the verge of mechanical stability and are called isostatic. Common isostatic lattices include the two-dimensional square and Kagome lattices as well as the three-dimensional cubic lattice with nearest-neighbor sites connected by central-force springs of spring constant $k$ and randomly packed spheres at random close packing at what is called point $J$. We calculate the phonon response functions and spectra of nearly isostatic square, cubic, and Kagome lattices in which springs of spring constant $k'$ connect next-nearest-neighbor sites. These lattices exhibit highly anisotropic modes at $k' = 0$, among which are soft modes with one-dimensional dispersion in wavenumber, giving rise to a flat density of states as a function of frequency $\omega$. In the square lattice, these modes are shear acoustic phonons, whereas in the Kagome lattice, they are optical phonons. When $k' > 0$, the low-energy modes crossover from acoustic phonons of the appropriate lattice symmetry for $\omega < \omega^* \sim \sqrt{d}$ to the soft isostatic-like modes for $\omega > \omega^*$, and the density of states crosses over from Debye-like to flat. Static phonon response functions exhibit correlation lengths $\xi \sim 1/\sqrt{d}$. We discuss the relation of these results to those for jammed systems near point $J$.

5:18PM T14.00015 Soft modes and elasticity of nearly isostatic lattices: randomness and dissipation, XIAOMING MAO, TOM LUBENSKY, Department of Physics and Astronomy, University of Pennsylvania — Isostatic periodic lattices, such as the square and Kagome lattices in spatial dimension $d = 2$, are systems at the onset of rigidity. They are marginally stable with coordination number $z = 2d$, and they may exhibit an non-extensive number of soft modes that can be removed by adding an infinitesimal number of additional bonds. Randomly packed frictionless spheres at the jamming point $J$ represent an important isostatic system that, because of its randomness, exhibits complexities beyond those of periodic systems. To study the effects of randomness on phonon response, propagation, and damping, we constructed model lattices near isostaticity by adding randomly distributed nearest-neighbor and second-nearest neighbor bonds to the isostatic square and kagome lattices, respectively. We calculated a number of properties of these models using the CPA approximation and found them to resemble those of jammed solids near the point $J$. In particular, the phonon density of states crosses over from Debye-like at low frequency $\omega$ to the flat frequency-independent behavior of a one-dimensional systems at a characteristic frequency $\omega^*$ that scales as the density of additional random bonds $\Delta z$. The real and imaginary part of the effective random-bond spring constants become equal at $\omega^*$. We also identify a characteristic length that scales as $(\Delta z)^{-1}$

Wednesday, March 18, 2009 2:30PM - 5:30PM — Session T15 DFD: Fluidic Devices: Micro and Nano 316

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2Supported by NSF grant DMR-0520020 and NSF grant DMR-080488 (AGY) helped support this research.

3This work was supported by NSF under grant No. DMR 0804900.
2:30PM T15.00001 Time evolution of distributive entropy in rectangular microchannel mixers, MIRON KAUFMAN, PETRÚ FODOR, Cleveland State University — Patterning ridges on the surface of microchannels has been found to be a viable strategy to induce mixing in straight channels, despite the characteristically small Reynolds numbers. In this work we evaluate the time evolution of the Rényi entropy associated with the spatial distribution of traces advected by an incompressible fluid moving in several straight rectangular channels: staggered herring bone [1], fractal surface patterning [2]. The steady state flow fields are obtained by solving the Navier – Stokes and continuity equations using a finite element analysis package. The Rényi entropy is then evaluated at different times using the spatial distribution of the tracers. The entropy increases with time as Int with a slope approximately equal to unity. The slope quantifies the rate of distributive mixing. The rate of increase in the entropy is found to be independent of the Rényi parameter. This is qualitatively different than the distributive mixing in channels with moving walls [3] where the rate of distributive mixing changes with the beta parameter. We also study the dependence of the distributive entropy on the Reynolds number. [1] A.D. Stroock et al., Science 295, 647 (2002); [2] M. Camesasca, M. Kaufman, I. Manas-Zloczower, J. Micromech. Microeng. 16, 2298 (2006); [3] W. Wang, I. Manas-Zloczower, M. Kaufman, Chemical Engineering Communications, 192(4), 405-423 (2005).

2:42PM T15.00002 Capillary absorption of metal nanodroplets by carbon nanotubes, SHAUN HENDY, Industrial Research Ltd, DMITRI SCHEBACHOV, Victoria University of Wellington — We present a simple model that demonstrates the possibility of capillary absorption of non-wetting liquid nanoparticles by carbon nanotubes assisted by the action of the Laplace pressure due to the droplet surface tension. We test this model with molecular dynamics simulation and find excellent agreement with the theory, which shows that for a given nanotube radius, there is a critical size below which a metal droplet will be absorbed. We then consider the dynamics of capillary absorption using the steady-state flow model due to Marmur, which is based on the Lucas-Washburn model with the addition of a driving force due to the Laplace pressure of the droplet. We find an exact solution to Marmur’s evolution equation for the height of the absorbed liquid column as a function of time, and show that this reproduces the dynamics observed in the simulations well. The simulations show that the flow of the metal exhibits a large degree of slippage at the tube walls, with slipp lengths of up to 10nm. These findings suggest new methods for fabricating composite metal-CNT materials, and have implications for our understanding of the growth of CNTs from metal catalyst particles. The results also explain the recent observations of the absorption of Cu nanodroplets by carbon nanotubes.

2:54PM T15.00003 Dynamic Pattern Formation In a Bubble-Generating Concentric Microfluidic Device, KENG-HUI LIN, KUO-YUAN CHUNG, Institute of Physics, Academia Sinica, Taipei, Taiwan — We observe rich spatiotemporal patterns of bubbles inside liquid droplets through a concentric microfluidic device made by two capillary tubes filled with gas and liquid respectively. When the gas pressure increases, the bubbles change from monodisperse, bimodal to polychr. The bubble size, the diameter of the bubbles can be scaled with the ratio of gas flow rate to the liquid flow rate. Our device offers different geometry to understand the bubble breakup in the microfluidic device.

3:06PM T15.00004 Flow-Based Organization of Soft Matter in Three Dimensions, LIAN LENG, SIVAISH ASLANBEIGI, AXEL GUENTHER, University of Toronto — Flows of miscible and immiscible liquids through microchannel networks have been previously used to achieve spatial organization within one plane. However, extending this approach to three dimensions, an essential requirement to create synthetic bulk materials with a regular microstructure, is not straightforward. To our knowledge for the first time, we demonstrate microfluidic strategy for the three-dimensional organization of soft bulk materials. The approach is enabled by a massively scaled microfluidic architecture that distributes two miscible or immiscible fluid streams through an array of parallel channels. The soft-lithographic fabrication process was adapted to consistently define microfluidic channel networks in elastomer substrates that are only 500 microns thick; followed by subsequent bonding of up to ten such layers in the vertical direction. The chip was connected with fluidic inlets, completely immersed in water and continuously extruded the organized material at its exit. Upon leaving the chip, neighbouring fluid streams formed a hydrogel retaining the desired regular microstructure. The material microstructure was controlled by adjusting the flow rates of the interdiffusing fluid streams (e.g. aqueous alginate and calcium chloride solutions).

3:18PM T15.00005 Viscous droplet deformation and breakup in microfluidic cross-flows, THOMAS CUBAUD, Stony Brook University — The dynamic response of translating high-viscosity droplets is experimentally investigated by means of a sharp increase of the flow velocity in a microchannel junction. The additional local injection of the continuous phase from symmetric side-channels into a square microchannel produces a broad range of time-dependent deformations and breakup. In particular, due to microscale wall confinement, the system displays a non-linear behavior with the initial droplet size. Deformations, relaxation times, and fragmentation processes are examined as a function of flow and fluids properties with a particular emphasis on the formation of slender viscous structures and spoon-like droplets, i.e., asymmetrical droplets.

3:30PM T15.00006 Morphology of liquids spreading along open nanofluidic channels, ANTONIO CHECCO, Brookhaven National Laboratory — Dynamic atomic force microscopy (AFM) in the non-contact regime is used to study the morphology of a non-volatile liquid (squalane) as it spreads along wettable nanostripes embedded in a non-wettable surface. AFM allows the direct observation of the microscopic contact line of spreading nanoliquids with unprecedented spatial resolution. Results show that the liquid profile depends on the amount of lateral confinement imposed by the nanostripes and it is truncated at the microscopic contact line in good qualitative agreement with classical mesoscale hydrodynamics. However, the width of the contact line is found to be significantly larger than expected theoretically. This behavior may originate from small chemical inhomogeneity of the patterned stripes as well as from thermal fluctuations of the contact line.

3:42PM T15.00007 Separation of chiral objects by shear flow in microfluidic channels - Theory, HENRY FU, Brown University — Dynamic atomic force microscopy (AFM) in the non-contact regime is used to study the morphology of a non-volatile liquid (squalane) as it spreads along wettable nanostripes embedded in a non-wettable surface. AFM allows the direct observation of the microscopic contact line of spreading nanoliquids with unprecedented spatial resolution. Results show that the liquid profile depends on the amount of lateral confinement imposed by the nanostripes and it is truncated at the microscopic contact line in good qualitative agreement with classical mesoscale hydrodynamics. However, the width of the contact line is found to be significantly larger than expected theoretically. This behavior may originate from small chemical inhomogeneity of the patterned stripes as well as from thermal fluctuations of the contact line.

3:54PM T15.00008 Separation of chiral objects by shear flow in microfluidic channels - Experiment, MARCOS, Massachusetts Institute of Technology, HENRY FU, THOMAS POWERS, Brown University, ROMAN STOCKER, Massachusetts Institute of Technology — We use microfluidics to test the prediction that a helix in shear flow drifts across streamlines. We use the non-motile, helical-shaped bacterium Leptospira biflexa as our model chiral object. As the shear in the top and bottom halves of the microchannel has opposite sign, we predict and observe the bacteria in these two regions to drift in opposite directions. The magnitude of the separation is in good agreement with theory.
4:06PM T15.00009 Tunable liquid optics: electrowetting-controlled liquid mirrors based on self-assembled Janus tiles, TOM KRUPENKIN, University of Wisconsin - Madison, MIKE BUCARO, Harvard University, PAUL KOLODNER, Bell Laboratories, ASHLEY TAYLOR, University of Wisconsin - Madison, ALEX SIDORENKO, University of the Sciences in Philadelphia, JOANNA AZENBERG, Harvard University — In this work we describe a tunable, high-reflectivity optofluidic device based on self-assembly of anisotropically-functionalized hexagonal micromirrors (Janus tiles) on the surface of an oil droplet to create a concave liquid mirror. The liquid mirror is deposited on a patterned transparent electrode that allows the focal length and axial position to be electrically controlled. The mirror is mechanically robust and retains its integrity even at high levels of vibrational excitation of the silica substrate. The use of reflection instead of refraction allows the limited available refractive-index contrast between pairs of density-matched liquids, allowing stronger focusing than is possible for a liquid lens of the same geometry. This approach is compatible with optical instruments that could provide novel functionality – for example, a dynamic 3D projector, i.e., a light source which can scan an image onto a moving, non-planar focal surface. Janus tiles with complex optical properties can be manufactured using our approach, thus potentially enabling a wide range of novel optical elements.

4:18PM T15.00010 A CMOS / Microfluidic Vesicle Based Lab-on-a-Chip Platform, DAVID ISSADORE, THOMAS FRANKE, KEITH BROWN, Harvard University, School of Engineering and Applied Sciences, ROBERT WESTERVELT, Harvard University, School of Engineering and Applied Sciences and Physics — Droplet based microfluidic systems have proved to be useful tools for performing lab-on-a-chip experiments. Our lab has designed CMOS / microfluidic chips to trap, move, and separate droplets of water in oil using dielectrophoresis (DEP) [1]. Vesicles provide a robust container for cells, bacteria, viruses, fluorescent markers, and can withstand a wide range of chemicals, salinity, and pH. We present a platform for programmable chemical and biological experiments that traps, moves, and merges vesicles suspended in water using DEP on our hybrid chip. Vesicles are loaded with 1.4mM NaCl and rhodamine and are suspended in a 200mM glucose solution. We trap and move individual vesicles along programmable paths at speeds up to 70 micrometers/sec. Two vesicles may be brought together and merged into one when triggered with electric fields that are created by the chip. [1] TP Hunt, D Issadore, RM Westervelt - Lab on a Chip, 2008.

4:30PM T15.00011 Designing actuated cilia pumping fluids in microchannels, ALEXANDER ALEXEEV, Georgia Institute of Technology, JULIA YEOMANS, University of Oxford, ANNA C. BALAZS, University of Pittsburgh — Using three-dimensional computational modeling, we examine the motion of actuated cilia in a fluid-filled microchannel. The cilia are modeled as deformable, elastic, filaments, which are initially tilted with respect to the channel surface. A sinusoidal force normal to the microchannel wall is applied at the free ends of the tilted cilia and induces periodic oscillations of these flexible filaments. To capture the complex fluid-structure interactions among these filaments, the channel walls and the surrounding solution, we employ our hybrid computational approach that combines a lattice Boltzmann model for hydrodynamics of viscous fluids and a lattice spring model for the micromechanics of elastic solids. We find that the actuated cilia give rise to a unidirectional flow in the microchannel and by simply altering the frequency of the applied force, we can control the direction of the net flow. The findings suggest that beating elastic cilia could be harnessed to regulate the fluid streams in microfluidic devices.

4:42PM T15.00012 A Deterministic Microfluidic Ratchet, KEVIN LOUTHERBACK, JASON PUCHALLA, ROBERT AUSTIN, JAMES STURM, Princeton University — We present a deterministic microfluidic ratchet where the trajectory of particles in a certain size range is not reversed when the sign of the driving force is reversed. This ratcheting effect is produced by employing triangular rather than the conventionally circular posts in a post array that systematically directs particles transported through the array. The underlying mechanism of this method is shown to be an asymmetric fluid velocity distribution through the gap between triangular posts that results in different critical particle sizes depending on the direction of the flow.

4:54PM T15.00013 Topological Dependence of ds-DNA Confined in Nanoslits, PO-KENG LIN, Institute of Atomic and Molecular Science, Academia Sinica, JEN-FANG CHANG, Institute of physics, Academia Sinica, CHENG-HUNG WEI, PEI-KUEN WEI, Research Center for Applied Sciences, Academia Sinica, Y.-L. CHEN, Institute of physics, Academia Sinica — Topological constraints are important for the DNA condensation in confinement, such as chromosome in the cell and bacteriophage DNA packaging. We investigated the topological dependence of the size, shape and diffusivity of λ-DNA confined in a nanoslit with height $h = 780 \text{ nm}$ (≈ bulk radius of gyration of λ-DNA) to strong confinement ($h = 20 \text{ nm} << Kuhn$ persistence length $\lambda$). Shape asphericity of both linear and circular DNA increases with decreasing $h$, which indicate the DNA become more anisotropic. Furthermore, we observed the transition from de Gennes to Odijk scaling in the measured extension and diffusivity when $h = Kuhn$ length $L_k$. Interestingly, the diffusivity of circular DNA is larger than linear DNA in the blob regime, but they are nearly equal in slits with $h << L_k$.

5:06PM T15.00014 Propagation modes of entropically trapped and extended DNA molecules, MORTEN MIKKELSEN, Technical University of Denmark, WALTER REISNER, Brown University, HENRIK FLYVBJERG, ANDERS KRISTENSEN, Technical University of Denmark — Nanofluidic systems are a powerful tool for controlling polymer conformation and dynamics in lab-on-a-chip type devices for the analysis of DNA and other biomolecules. We present a new device concept that combines confinement-based extension of DNA with the entropic trapping principle, leading to qualitatively new physics and applications. The device consists of a 50 nm slit channel with an array of transverse $100 \times 100 \text{ nm}$ grooves, where the transport of DNA molecules perpendicular to the groove axis is investigated under pressure driven buffer flow. At low flow velocities the DNA remains trapped and extended in the nanogrooves while buffer circulates through the slit, enabling physical mapping of the DNA while performing real time buffer exchanges. For flow velocities above a molecular weight dependent escape threshold, we show that the transport process through the slit channel randomly alternates between two modes of propagation: A stepwise groove to groove hopping, called the ‘sidewinder’, and a continuous tumbling across the grooves, where the molecules feel the topology as an effective friction, called the ‘tumbleweed’. The observed length dependence on the molecule velocity may lead to a novel separation methodology.

5:18PM T15.00015 Multiplex selection and elution of aptamers using nanoporous sol-gel droplets and a microheater array, SEUNG-MIN PARK, Cornell University, JIYOUNG AHN, MINJOUNG JO, SOYOU N KIM, Dongguk University, DONG-KI LEE, Sungkyunkwan University, JOHN LIS, PANGSHUN ZHU, HAROLD CRAIGHEAD, Cornell University — Aptamers are well-known protein capture reagents that bind to specific proteins and can be effective in inhibiting the protein’s normal interactions. Here, we have described a process for selective binding and elution of aptamers from the nanoporous silicate sol-gel droplets within which target proteins are immobilized. These silicate sol-gel droplets are incorporated with polydimethylsiloxane (PDMS) microfluidic systems and individually addressable by electrical microheaters. These properties allow discrete protein – nucleic acids interaction so that multiplexed selection is possible. It is shown that specific aptamers bind their respective protein targets and can be selectively eluted by micro-heating. Our microfluidic in vitro selection system improves selection efficiency, reducing the number of selection cycles needed to produce high affinity aptamers. We are also able to separate high-affinity nucleic acid species from a large random nucleic acid pool. The process is readily scalable to larger arrays of sol-gel-embedded proteins.

Thursday, March 19, 2009 8:00AM - 10:36AM – Session V14 DFD GSNP: Disordered Systems, Glassy Dynamics, and Jamming II
8:00AM V14.00001 Specific Heat Anomalies in Glassy Fluids Due to Cluster Micro-Melting.

GEORGE HENTSCHEL, Emory University, VALERY ILYIN, ITAMAR PROCACCIA, NURITH SCHUPPER, Weizmann Institute of Science — We will discuss the specific heat anomalies observed in new simulations of equimolar mixtures of particles interacting via soft core repulsive potentials under external pressure that are known to show glassy dynamics at low temperatures. The simulations show both long-lived states of microcrystalline clusters that do not nucleate a crystalline ground state and also the appearance of two specific heat peaks which were not observable in earlier simulations. We argue that the appearance of two peaks is due to the micro-melting of two types of clusters and discuss the form of the resulting specific heat anomalies. Our arguments suggest that the glass transition will typically show non-universal features.

8:12AM V14.00002 The building blocks of Dynamical Heterogeneities in dense granular media.

Raphael Canelier, Olivier Dauchot, Giulio Biroli, CEA — Unveiling the connection between the short term relaxation and the long term dynamical heterogeneities as observed near the glass transition in super-cooled liquids and the jamming transition in granular materials remains a major challenge in the physics of glassy systems. On one hand, KMC models relate dynamical heterogeneities to a non trivial structure in the trajectory space, inherited from the local dynamical rules. On the other hand, recent studies of hard spheres close to isostaticity suggest that the collective aspect of the relaxation would stem from the extended character of the softest degrees of freedom, along which the system yields from one meta-basin to another. There is still no direct experimental evidence in favour of one or the other mechanism in super-cooled liquids nor in dense granular media. Here we will show that for a dense granular layer under cyclic shear dynamical heterogeneities result from a two timescales process. Short time but already collective events consist in clustered cage jumps, which concentrate most of the non affine displacements. Such clusters aggregate both temporally and spatially within an avalanche process, which ultimately builds the large scales dynamical heterogeneities. The typical timescale of the dynamical heterogeneities appears as the crossover between the short time separating successive event within the avalanches and the long time separating the successive jumps of any given particle.

8:24AM V14.00003 Role of Shape Anisotropy on the Glassy Dynamics of Colloidal Suspensions.

Mukta Tripathy, Kenneth Schweizer, University of Illinois, Urbana-Champaign — Center-of-mass ideal mode coupling theory (MCT), the nonlinear Langevin equation (MCT), the Reference Interaction Site Model have been employed to model the structure and slow dynamics of suspensions composed of hard and rigid nonspherical particles. Objects of dimensionality one (rods, rings), two (discs), and three (polyhedra) have been studied. For non-compact particles the volume fraction of ideal kinetic arrest, corresponding to a crossover to activated dynamics, decreases with particle dimensionality and/or aspect ratio. On the other hand, the ideal vitrification volume fraction of compact 3-dimensional objects is a complex and subtle function of particle shape. Calculations of the entropic barrier for activated transport, mean relaxation time, transient localization length, diffusion constant, elastic modulus, and effective fragility have been performed. Deep in the ideal glassy region the barrier height and mean hopping time are controlled by the shape-dependent mean square confining force exerted on a particle by its surroundings. A nearly universal collapse of many dynamical properties is achieved based on a dimensionless difference variable that quantifies the magnitude of the mean square force compared to its critical value at the ideal MCT transition.

8:36AM V14.00004 Coupled Translational and Rotational Glassy Dynamics in Hard Dicolloid Suspensions.

Rui Zhang, Kenneth Schweizer — Naive mode coupling theory (NMCT) and the nonlinear Langevin equation (NLE) theory of activated glassy dynamics have been generalized to treat the coupled center-of-mass translation and rotational motions of hard linear objects of variable aspect ratio. Two types of ideal nonergodicity transitions are predicted corresponding to localization of only translation (plastic glass for small aspect ratios) or simultaneous arrest of translation and rotation (double glass). The NMCT kinetic arrest transition signals a crossover to activated dynamics controlled by entropic barriers. Specifically, a two-dimensional dynamical free energy surface (function of translational displacement and rotational angle) is constructed which quantifies effective rates for all aspect ratios the most efficient activated process corresponding to the trajectory of lowest entropic barrier is associated with a system-specific translation-rotation cooperative motion. Mean alpha relaxation times as a function of dicolloid aspect ratio and volume fraction are computed using multidimensional Kramers theory.

8:48AM V14.00005 Constitutive relations in dense granular flows.

John Drozd, Colin Denniston, University of Western Ontario — We use simulations to investigate constitutive relations in dry granular flow. Our system is comprised of mono- and poly-disperse sets of spherical grains falling down a vertical chute under the influence of gravity. We observe three phases or states of granular matter: a free-fall dilute granular gas region at the top of the chute, a granular fluid in the middle and then a glassy region at the bottom. We test various proposed constitutive relations to provide a basis for analytically solving for the stresses in granular flows. Finally, we examine the energy conservation and heat flow in our systems and show that the heat conductivity constitutes distinct power-law dependences on the granular temperature in the glassy and fluid regions of our system.


Patrick Charbonneau, Duke University, Jacobus A. Van Meel, FOM Institute for Atomic and Molecular Physics, Daan Frenkel, Cambridge University — Geometrical frustration is thought to ease the supercooling of a liquid. In 3d hard spheres the preferred local cluster isicosahedral and the densest packing is tetrahedral, but no periodic lattice is consistent with either symmetry in Euclidian space, so a crystal phase with a different symmetry nucleates upon compression. For 2d disks in contrast triangular or hexagonal order is both locally and globally preferred and crystallization of a metastable fluid is quasi-instantaneous. Yet the precise origin of geometrical frustration remains unclear, because in 2d and 3d polytetrahedral structures are often equated conceptually to the optimal local cluster. Here, we conduct a computational study of the 4d analogue, where the optimal local cluster and global order are commensurate, but the polytetrahedral order is not. We observe no sign of facile crystal formation, which supports the polytetrahedral frustration scenario. We also find the fluid to be structurally very different from the crystal. The resulting high interfacial free energy sheds new light on 3d geometrical frustration and its role in glass formation.


Zhi Chen, Clare Yu, University of California, Irvine — Noise is ubiquitous and and is often viewed as a nuisance. However, we propose that noise can be used as a probe of the fluctuations of microscopic entities, especially in the vicinity of a phase transition. In recent work we have used simulations to show that the noise increases in the vicinity of phase transitions of ordered systems. We have recently turned our attention to noise near the phase transitions of disordered systems. In particular, we are studying the noise near Ising spin glass transitions using Monte Carlo simulations. We monitor the system as a function of temperature. At each temperature, we obtain the time series of quantities characterizing the properties of the system, i.e., the energy and magnetization. We look at different quantities, such as the noise power spectrum and the second spectrum of the noise, to analyze the fluctuations.


Vijayakumar Chikkadi, University of Amsterdam, The Netherlands, Andrew Schofield, University of Edinburgh, U.K., Peter Schall, University of Amsterdam, The Netherlands — We perform slow shear of colloidal glasses using a confocal microscope and shear-cell set up. The particles are tracked in time and space to construct the local strain field, which is observed to be non-uniform with high strain and low strain zones interspersed in space. Our measurements at a volume fraction ~ 59% show the existence of homogeneous sheared regime, at a shear rate ~5x10^{-5} s^{-1} and shear localization at higher shear rates (~10^{-4} s^{-1}). The set-up offers a unique opportunity to elucidate the evolution of shear-bands using the concept of shear transformations. In particular, the aim is to understand the role of correlation between the shear transformations in the growth of shear bands. We present an overview over the homogeneous versus inhomogeneous shear regime in terms of a deformation map for these systems.

Work supported by DOE grant DE-FG02-01ER46107.
Correlations between Dynamical Heterogeneity and Viscoelasticity of Confined Colloidal Suspensions under Oscillatory Shear, PRASAD SARANGAPANI, YINGXI ELAINE ZHU, University of Notre Dame, Department of Chemical and Biomolecular Engineering, Notre Dame, IN 46556 — In this talk, we present a recent rheological study of confined amorphous colloidal thin films under oscillatory shear using a home-designed micron-gap rheometer interfaced with a confocal microscope. We visualize the response of “hard-sphere” poly-(methyl methacrylate) (PMMA) particles of 1.2 µm in diameter to applied shear deformation and simultaneously measure the viscous and elastic moduli of PMMA colloidal thin films of bulk volume fraction, φ = 0.43-0.57, confined at gaps ranging from 50 µm to 1-2 µm. For confined PMMA colloids under shear at gaps where an applied deformation is sufficiently large to induce non-linear responses, we find commonality in particle dynamics where strongly non-affine motion causes particles to move as cooperatively rearranging groups. However, on average the length scale of these groups is larger than the typical length scales of dynamical heterogeneities for the un-sheared thin films and typically approaches the order of confining dimension. We quantify the nature of shear induced flow cooperativity and its relation to a shear thickening transition observed in the limit of large strain amplitudes.

Aggregation of athermal particles induced by capillarity, MICHAEL BERHANU, ARSHAD KUDROLLI, Department of Physics, Clark University, Worcester, MA 01610 — Aggregation of cohesive particles floating in a medium is a very broad physical phenomena occurring in colloidal systems, soot particles, and intergalactic dust under gravitation. We investigate the geometrically constrained dynamics of aggregation with new experiments using floating spheres at the air-liquid interface. A short range attractive force can be induced by careful choice of buoyancy and capillarity to create self-assembled particle structures which can be tracked by imaging. First, the particles are placed randomly at the interface, and then aggregation is induced by smoothly decreasing the area of the interface which causes the particles to come within the attractive force range caused by capillarity. We measure the area fraction at which the connectivity and rigidity percolation transitions are observed and further characterize the aggregates with two-point correlation functions. We then compare and contrast our results with gelation and jamming transitions reported with colloids and granular matter. Finally, we study the reverse phenomena, where we probe the response of the aggregate to an increase in interface area.

Correlation range in a supercooled liquid via Green-Kubo expression for viscosity, local atomic stresses, and MD simulations, VALENTIN A. LEVASHOV, TAKESHI EGAMI, JAMES R. MORRIS, University of Tennessee and Oak Ridge National Laboratory — We present a new approach to the issue of correlation range in supercooled liquids based on Green-Kubo expression for viscosity. The integrand of this expression is the average stress-stress autocorrelation function. This correlation function could be rewritten in terms of correlations among local atomic stresses at different times and distances. The features of the autocorrelation function decay with time depend on temperature and correlation range. Through this approach we can study the development of spatial correlation with time, thus directly addressing the question of dynamic heterogeneity. We performed MD simulations on a single component system of particles interacting through short range pair potential. Our results indicate that even above the crossover temperature correlations extend well beyond the nearest neighbors. Surprisingly we found that the system size effects exist even on relatively large systems. We also address the role of diffusion in decay of stress-stress correlation function.

Dynamics in Complex Fluids Formed by Conjugated Polymers, NARESH OSTI, Department of Chemistry, Clemson University, Clemson, SC 29634, MADHUSUDAN TYAGI, NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD 20899, DILRU RATNAWEERA, Department of Chemistry, Clemson University, Clemson, SC 29634, UWE BUNZ, Department of Chemistry and Biochemistry Georgia Institute of Technology, Atlanta, GA 30332, DVORA PERAHIA, Department of Chemistry, Clemson University, Clemson, SC 29634 — Alkyl di-substituted para-polyphenyleneethylen (PPE) associates into several complex fluids in dilute solutions of toluene. At high shear stress the molecules assemble into a supercooled liquid. As the temperature decreases the molecules associate and eventually jam to a fragile gel. These phases are optically active where the dynamic processes affect their optical characteristics. Inelastic Neutron Back Scattering conjunction with Neutron Spin Echo was used to characterize the dynamics on multiple length scales at different temperatures. The current talk will introduce the neutron backscattering results that follow internal dynamics within the PPE molecules as they are confined into aggregates and jams to form a fragile phase. The data will be discussed in terms of Kohlrausch-Williams-Watt model that provides characteristics time constants for the different dynamic processes.

Spontaneous transition in TiNiFe strain glass system, JIAN ZHANG, XIAOBING REN, YU WANG, KAZUHIRO OTSUKA, JUN SUN, Multi-disciplinary Materials Research Center, Xi an Jiaotong University,710049, P.R. China. Ferroic physics group, NIMS, Tsukuba, Japan — Glass has been considered as one major challenge for the statistic mechanics, for the presumption of ergodicity is no longer valid. Hence, glass transition was normally viewed as solely kinetic driven process, including ferroic cluster glasses. Whereas, the ferroic cluster glasses appear once the thermodynamics driven ferroic phase transitions are suppressed by the point defects. It seems quite intriguing why the power of thermodynamics is immediately eliminated when the system reaches the threshold composition, and taken over completely by kinetics. We demonstrate the power of the thermodynamics on the glass state by presenting for the first time the existence of spontaneous transition from strain glass to long range phase in the newly found strain glass in TiNiFe, evidenced with various experimental methods. In addition, we provide one phenomenological model to reveal the underlying mechanism due to the competition between the thermodynamic and kinetic factors. Our results on this relatively simply glass system may bring new ideas in other fields of science and technology, i.e. biophysics and biochemistry.

Thursday, March 19, 2009 8:00AM - 10:48AM —
Session V15 DFD: Liquid Crystals

Interaction and Response of a Smectic-A liquid crystal to a 2 nm Nanoparticle Phase transition due to the Functionalization Compound, LUZ J MARTINEZ-MIRANDA, University of Maryland, LYNN K KURIHARA, Naval Research Laboratories — We have studied the in-plane (parallel to the magnetic field) alignment of 8CB mixed with FeCo nanoparticles covered with different functionalization compounds. The functionalization compounds are Polyethylene glycol (PEG (3000)), hydroxyl succinimide (NHS), aminopropyl tri-ethoxy silane (APTS) and mercapto hexa-decanoic acid (MHDA). We have studied them using X-ray scattering. We have found that the nanoparticles, functionalization compound) will need to reorient the liquid crystal in the magnetic field. In addition, we have observed that the orientation the liquid crystal adopts with respect to the nanoparticles can result in a phase transition that takes the liquid crystal to a more disordered and symmetric phase. Finally, we study the reverse phenomena, where we probe the response of the aggregate to an increase in interface area.
8:12AM V15.00002 Theory of Ferroelectric Nanoparticles in Nematic Liquid Crystals1, LENA LOPATINA, JONATHAN SELINGER, Liquid Crystal Institute, Kent State University — Many recent experiments have reported that ferroelectric nanoparticles have drastic effects on nematic liquid crystals. Low concentrations of such particles increase the nematic-isotropic transition temperature by over 10°C, and greatly increase the sensitivity of the nematic phase to applied electric fields. To understand these effects, we develop a theory for the statistical mechanics of ferroelectric nanoparticles in liquid crystals. In this theory, the key issue is the distribution of orientations for the electrostatic dipole moments of the nanoparticles. This distribution is characterized by an orientational order parameter, which interacts with the orientational order of the liquid crystals and stabilizes the nematic phase. We estimate the coupling strength and calculate the resulting enhancement in the transition temperature, in good agreement with experiments. We also predict the response to applied electric fields, showing that the Kerr effect is enhanced above the isotropic-nematic transition. These predictions apply even when the electrostatic interactions are partially screened by moderate concentrations of ions.

1This work was supported by NSF Grant DMR-0605889.

8:24AM V15.00003 Unconventional dimerization in mesogenic semi-phasmidic type carboxylic acid*, SHIN-WOONG KANG, SEUNG-YEON JEONG, DENA MAE AGRA-KOOLJMAN, SATYENDRA KUMAR, Department of Physics, Kent State University, VEENA PRASAD, SANJAY VARSHNEY, Centre for Liquid Crystal Research, Bangalore, INDIA — The nematic and columnar mesophases formed by a semi-phasmidic type carboxylic acid are investigated by DSC, X-ray scattering, FTIR spectroscopy, and polarizing optical microscopy. FTIR spectroscopy and X-ray results confirm that two semi-phasmidic type carboxylic acid molecules form a mesogenic dimer through inter-molecular hydrogen bonding. X-ray diffraction results obtained under in-situ magnetic field reveal unique characteristics that set them apart from conventional linear dimers formed via hydrogen bonding. These dimers possess negative dielectric and diamagnetic anisotropies. Values of the length scales corresponding to the diffraction peaks and their orientation relative to the magnetic field strongly suggest the formation of a “bent-core-like” mesogenic dimers rather than conventional coplanar linear dimers.


8:48AM V15.00005 The shape and conformation of the mesogenic group in tetrapodic liquid crystals1, HYUNG YOUNG YOON, SHINWOONG KANG, Department of Physics, Kent State University, GEORGE H. MEHL, Department of Chemistry, University of Hull, UK, SATYENDRA KUMAR, Department of Physics, Kent State University — The nematic phases formed by tetrapodic mesogens based on Si- or Ge- core have been investigated by various methods [1]: deuterium NMR, polarized IR spectroscopy, and light scattering. In these studies, biaxiality of the nematic phase has been the central issue. The average structural shape of such a complex molecule adopts and how the four mesogens attached to Si/Ge atom are oriented in the nematic and lower temperature phases are naturally important questions. However, these have not been sufficiently discussed. We performed synchrotron x-ray diffraction experiments on magnetic aligned Ge-tetrapodes, augmented by conoscopy, capacitance, and electro-optical experiments. The results of these studies and the inferences drawn for the mesogenic group formation will be presented. [1] K. Neupane, S.W. Kang, S. Sharma, D. Carney, T. Meyer, G. H. Mehl, D.W. Allender, S. Kumar, and S. Sprunt, Phys. Rev. Lett. 97, 207802 (2006), and references there in.

1Supported by grant NSF/DMR-080991.

9:00AM V15.00006 Quantum dot dispersion in nematic liquid crystal, J. KIRCHHOFF, Florida State University, R.H. INMAN, D.S. CHANDHOK, S. GHOSH, L.S. HIRST, University of California Merced — Optical and electrical properties of quantum dots can be significantly altered by aligning the dots in a linear chain. Dispersing quantum dots in liquid crystals can lead to the formation of linear chains due to the partial ordering of the liquid crystal molecules. Typically, this results in a red shift in the emission spectrum of the dots as the induced order leads to enhanced dipolar interactions, resulting in electronically coupled states. Dispersions of quantum dots are studied as a function of the concentration, size, and shape of the dots in a nematic rod-like liquid crystal material. The quantum dots are seen to aggregate if the concentration of the dots is too high, leading to enhanced dipolar interactions, resulting in electronically coupled states. Dispersions of quantum dots are studied as a function of the concentration, size, and shape of the dots in a nematic rod-like liquid crystal material. The quantum dots are seen to aggregate if the concentration of the dots is too high, leading to little correlation between the quantum dot dispersion and liquid crystal texture. In decreasing the quantum dot concentration the aggregates lessen in size and are more uniformly distributed within the liquid crystal. Spherical, rod-like, and disc-like quantum dots with emission peaks ranging from 490 nm to 640 nm were studied using polarized optical microscopy and scanning microscopy photoluminescence measurements.


1Supported by NSF Grant DMR-0504516 and DOE grant DE-FG02-06ER46331.

9:24AM V15.00008 Highly Oriented Neurofilament Liquid Crystalline Gels for Imaging and Scattering Studies, H. C. HOLGER, R. BECK, C. DING, J. B. JONES, J. DEEK, N. C. MACDONALD, Y. LI, C. R. SAFIYNA, UC Santa Barbara — The neuronal cytoskeleton is composed of a variety of filamentous proteins including, neurofilaments (NFs), microtubules (MTs) and actin. These components form networks that maintain the cell's structure and shape. At high filament concentration, the proteins self-assemble in vitro and form liquid crystalline phases maintained by their spatial anisotropy and interfilament interactions. Under physical confinement in microchannel with widths less than few persistence lengths, both MT and actin bundles align parallel to the surface. AFM imaging shows that despite being shorter and more flexible filamentous protein, NF networks maintain larger oriented domains over much longer length scales and unexpectedly align perpendicular to the microchannel walls. We discuss the extended orientation order in NFs in terms of the inter-filaments interactions originating from their polyampholyte side-chains. Supported by DOE DE-FG02-06ER46331, NSF DMR-0803103, and the Human Frontier Science Program organization. [1] N.F. Boussen et al., APL 85 (2004) 5775; L.S.Hirst et al. Langmuir 21 (2005) 3910 [2] H.C. Hesse, R. Beck, J. Deek et al. Langmuir 24 (2008) 8397
9:36AM V15.00009 Theory and simulation of two-dimensional nematic and tetragonal phases\textsuperscript{1}. JUN GENG, JONATHAN V. SELINGER, Liquid Crystal Institute, Kent State University — Recent experiments and simulations have shown that two-dimensional systems can form tetragonal phases with four-fold rotational symmetry, even if they are composed of particles with only two-fold symmetry. To understand this effect, we propose a model for the statistical mechanics of particles with almost four-fold symmetry, which is weakly broken down to two-fold. We introduce a coefficient $\kappa$ to characterize the symmetry breaking, and find that the tetragonal phase can still exist even up to a substantial value of $\kappa$. Through a Landau expansion of the free energy, we calculate the mean-field phase diagram, which is similar to the result of a previous hard-particle excluded-volume model. To verify our mean-field calculation, we develop a Monte Carlo simulation of spins on a triangular lattice. The results of the simulation agree very well with the Landau theory.

\textsuperscript{1}This work was supported by NSF Grant DMR-0605889.

9:48AM V15.00010 Quadrupolar particles in a nematic liquid crystal: Effects of particle size and shape. FRANCISCO HUNG, Cain Department of Chemical Engineering, Louisiana State University — We investigate the effects of particle size and shape on the quadrupolar (Saturn ring-like) defect structures formed by a nematic liquid crystal (NLC) around nm- and micron-sized particles with spherical, spherocylindrical, and cubic shapes. Our calculations, based on a Landau-de Gennes expansion in terms of the tensor order parameter $Q$, indicate that for pairs of nanoparticles in close proximity, the most stable defect structure is the “entangled hyperbolic” [1]. For pairs of micron-sized particles the NLC forms entangled “figure of eight” defects [1] around pairs of spheres and spherocylinders. In contrast, we only observed unentangled defect structures around pairs of micron-sized cubic particles. For pairs of spherical and spherocylindrical particles, the transition between “entangled hyperbolic” and “figure of eight” structures occurs when the particle diameter is between 100 nm and 1 micron. Our calculations suggest that the NLC-mediated interactions between the nanoparticles are fairly strong (up to 5700 kT). These interactions can bind the particles together at specific locations, and thus could be used to assemble the particles into ordered structures with different morphologies. [1] M. Ravnik et al., Phys. Rev. Lett. 99, 247801 (2007)

10:00AM V15.00011 A Model Liquid Crystalline System Based on Rodlike Viruses with Tunable Chirality, DANIEL BELLER, EDWARD BARRY, ZVONIMIR DOGIC, Brandeis University — Filamentous bacteriophages such as the fd virus have long been used as ideal model systems to investigate the phase behavior of suspensions of rodlike particles. We study the structure and phase behavior of a mutant, fd Y21M, and compare them to the properties of conventional fd wild-type (wt). These two viruses exhibit dramatically different phase behavior despite differing only by a single amino acid of the major coat protein pVIII. We find that this is attributable to significant differences in the flexibility of the viruses. Using the more rigid fd Y21M, we are able for the first time to quantitatively test the Ongser description of the isotropic-nematic phase transition of rigid rods. Even more surprising are the differences in the behavior of the cholesteric phase of fd Y21M and fd wt. While fd wt forms a cholesteric pitch with a left-handed helix, fd Y21M forms a cholesteric pitch with the opposite handedness. In addition, the magnitude of the cholesteric pitch changes by almost fivefold. Using mixtures of the two viruses, we are able to create liquid crystal systems with tunable control over the macroscopic chiral behavior.

10:12AM V15.00012 Apparent Broken Reciprocity in Chiral Liquid Crystals\textsuperscript{1}. MICHELE MOREIRA, NITHYA VENKATARAMAN, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University, LORENZO MARRUCCI, Dipartimento di Scienze Fisiche, Università di Napoli “Federico II” — Reciprocity in optics is predicated on bounded scattering media with symmetric and linear permittivity, conductivity and permeability. Due to their anisotropy and chirality, cholesteric liquid crystals (CLCs) form periodic dielectric structures. If the periodicity is comparable to the wavelength of light, these phases are self-assembled photonic band gap structures. There appear in the permittivity odd powers of the wave vector resulting from nonlocality and broken inversion symmetry. Evidence of non-reciprocity has been found in optically active crystals by Bennett [1] and in stacks of cholesteric and nematic liquid crystal cells by Takezoe [2]. We investigate experimentally and theoretically the possibility of a violation of optical reciprocity of a hetero-photonic-bandgap structure made of two CLC cells of different pitch. We have observed a significant apparent violation, but we show that the effect is due to light scattering, and in fact these cholesteric structures are reciprocal.


\textsuperscript{1}This work was supported by the AFOSR under MURI grant FA9550-06-1-0337.

10:24AM V15.00013 Raman scattering study of orientation order parameters in thermotropic biaxial nematic LC, MIN SANG PARK, BUM JIN YOON, JUNG OK PARK, School of Polymer, Textile and Fiber Engineering, Georgia Institute of Technology, Atlanta, GA, USA, VEENA PRASAD, Center for Liquid Crystal Research, Bangalore, India, MOHAN SRINIVASARAO, School of Polymer, Textile and Fiber Engineering, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA, USA — There has been considerable interest in the liquid crystalline phases formed by bent-core molecules, since these molecules were considered to have a biaxial nematic phase. In an effort to understand the orientation behavior and the degree of phase biaxiality in bent-core mesogens, Raman spectroscopy has been used to measure the scattering intensities for orthogonal linear polarization. This straightforward methodology allows the values of both uniaxial, $<P_{200}>$ and $<P_{400}>$, and biaxial order parameters, $<P_{220}>$, $<P_{210}>$, and $<P_{410}>$ to be quantified. From experimentally derived order parameters, the most probable orientation distribution functions are constructed. The results of these measurements will be presented in the context of experimental evidence of phase biaxiality obtained by other methods including X-ray diffraction and NMR.

10:36AM V15.00014 Liquid crystalline behaviors of H-bonded dimer formed from the semi-phasicmic type carboxylic acid*, SEUNG-YEON JEONG, SHIN-WOONG KANG, SATYENDRA KUMAR, Department of Physics, Kent State University, VEENA PRASAD, SANJAY VARSHNEY, Centre for Liquid Crystal Research, Bangalore, INDIA — Liquid crystalline properties of acid-functionalized semi-phasicmic azo-compound were characterized by DSC, polarizing optical microscopy, and electro-optical measurements. The results suggested that this unconventional mesogenic dimer has a non-typical effective “bend” angle where two monomers form the hydrogen bond. To confirm this we performed electro-optical experiments in the nematic phase with strong external electric and magnetic fields. Cells with different surface geometries and treatments we used. The results reveal a behavior that is very distinct from that expected of conventional linear mesogenic dimers formed by a hydrogen bonding. The results confirm negative values of dielectric and diamagnetic anisotropies. Our observations indicate that “bent-core-like” dimers mesogens are formed through an unconventional inter-molecular association. *Work supported by grant NSF/DMR-086991.
11:15AM W14.00001 Clustering in a Dense, Freely-Falling Granular Stream\(^1\), JOHN R. ROYER, SCOTT R. WAITUKAITIS, James Franck Institute, University of Chicago, DANIEL J. EVANS, HEINRICH M. JAEGER, James Franck Institute, University of Chicago — We investigate the breakup of a freely-falling granular stream into discrete, compact clusters of grains. This breakup, occurring for grain diameters less than about 200 microns falling out of a hopper opening, is reminiscent of the breakup of a liquid stream, though granular materials are generally thought of as lacking a surface tension. Our experiments employ high-speed video imaging in the co-moving frame, which allows us to track the onset of clustering and the subsequent cluster evolution in detail. Varying the material, size, roughness, and wetting properties of the grains as well as the surrounding gas pressure and the hopper opening diameter, we investigate the role of capillary, electrostatic and van der Waals forces in the clustering process. We find that the clustering provides a window to observe very weak cohesive forces between the grains which are masked in other experiments.

\(^1\)This work was supported by NSF through DMR-MRSEC and by the W. M. Keck Foundation

11:27AM W14.00002 Vector Force Measurements of a Dense Granular Flow\(^1\), KEVIN FACTO, University of Massachusetts-Amherst, TOM SCHICKER, NARAYANAN MENON, University of Massachusetts-Amherst — We have made force measurements at the wall of a dense granular flow. The data was acquired at a rate of 800 Hz in all three spatial directions. The fluctuations in the forces were examined for a wide range of flow speeds. Correlations in the forces decay by the time the flow moves one ball diameter. The force along the flow direction is highly correlated with the force normal to the wall. For a given value of normal force, the force along the flow has a gaussian distribution about the tangential force that would be predicted from a constant friction angle.

\(^1\)Supported by NSF DMR-0606216 and NSF CBET-0651397

11:39AM W14.00003 Space-Time Structure of Granular Flows in a Rough Vertical Channel\(^1\), DONALD CANDELA, KEVIN FACTO, University of Massachusetts Amherst — We report measurements using PFG-NMR of the space and time structure of steady granular flows through a long vertical channel of circular cross section with roughened walls. The granular sample consisted of seeds approximately 400 \(\mu\)m in diameter, flowing through a 9.8 mm ID tube to which was adhered a monolayer of glass beads similar in diameter to the grains. Data was acquired from a region approximately 50 channel diameters higher than the aperture at the channel bottom used to control the flow rate. The mean velocity of the grains as well as the RMS fluctuations in the grain motion were measured as functions of the radial coordinate and for time intervals in the range 5-200 ms, for several different granular flow speeds. For some flow regimes the displacement distributions are distinctly non-Gaussian, at odds with a “molecular fluid” model of the granular medium. The time dependence of the fluctuation distribution provides clues to the mechanism by which the gravitational body force is transmitted to the channel walls.

Supported by NSF DMR 0606216 and NSF MRSEC DMR 0213695

11:51AM W14.00004 Vibrheology of Granular Matter , JOSHUA DIJKSMAN, GEERT WORTEL, MARTIN VAN HECKE, Leiden University — We show how weak agitation substantially modify the rheology of granular materials. We experimentally probe dry granular flows in a weakly vibrated split bottom shear cell — the weak vibrations act as the agitation source. By tuning the applied stress and vibration strength, and monitoring the resulting strain, we uncover a rich phase diagram in which non-trivial transitions separate a jammed phase, a creep flow case, and a steady flow case.

12:03PM W14.00005 Shear zones at the walls of a 2D gravity-driven flow of grains\(^1\), KELSEY HATTAM,NALINI EASWAR, Smith College, Northampton, MA, NARAYANAN MENON, University of Massachusetts, Amherst, MA — We study the flow of spherical grains under gravity in a vertical, straight-walled 2-dimensional hopper, where the flow velocity is controlled by a taper at the outlet. We perform these studies both for monodisperse steel spheres as well as for a bidisperse system of equal numbers of spheres with a ratio of diameters of 1.25. The monodisperse system shows crystalline order even in flow, whereas there is no obvious structural order in the bidisperse system. The velocity profile across the flow is profoundly different in the two systems: the wall shear zone in the monodisperse system extends only a few particle diameters, and there are only small velocity gradients in the bulk of the flow. In contrast to this nearly-plug-like flow, there are significantly broader shear zones in the disordered flow. We report these profiles as a function of the width of the hopper in order to study the scaling of the shear zone with the system size, and with the flow rate.

\(^1\)Supported by NSF DMR 0606216 and NSF MRSEC DMR 0213695

12:15PM W14.00006 A Void Diffusion Model of Granular Flow , JAYANTA RUDRA, PAUL VIETH, Oklahoma School of Science and Mathematics — In an earlier paper we derived a nonlinear diffusion equation to describe the dynamics in granular flow based on a Diffusion Void Model (DVM). The equation was successfully used to describe the flow of a homogeneous granular material through the hole of a container under gravity. It also properly described similar flow in the presence of a flat horizontal barrier placed above the hole. Recently, however, we have found out that the above nonlinear equation does not lead to correct static equilibrium. For example, the stability of the free surface of a granular aggregate cannot be described by the equation. The equation also fails to describe, say, how an unstable vertical column of a granular material will change to a stable \(\Lambda\)-shaped pile at the angle of repose. In this paper we derive an equation using an appropriate current density of voids that can explain all the observed dynamical characteristics of a simple granular state. \(^1\)Jayanta K. Rudra and D. C. Hong, Phys. Rev. E47, R1459(1993).

12:27PM W14.00007 The Role of Extensional Viscosity in Sedimentation of Dense Suspensions , THEODORE BRZINSKI, DOUGLAS DURIAN, University of Pennsylvania — When two particles in a viscous fluid approach contact the motion of the interstitial fluid is dominated by extensional flows. We are interested in how the details of these flows influence the sedimentation of sense suspensions. To highlight the effects of extensional flows on particle motion we compare systems in which the fluids have the same shear viscosities, but drastically different extensional viscosities. We enhance the extensional viscosity by adding a flexible, high molecular weight polymer. In the case of a system without polymer there is a dense, static packing which grows from the bottom of the container, a region which remains at the initial grain density and settles at a constant velocity, and a clear supernatant at the top. In the polymeric fluid particles settle more slowly, and rather than sedimenting directly from the initial density to a static packing there is a long consolidation process during which the particle density increases at a constant rate.

12:39PM W14.00008 Local Rearrangements in a Dense Granular Medium During Steady and Oscillatory Shear , STEVEN SLOTTERBACK, University of Maryland: College Park, KRISZTIAN RONASZEGI, Budapest University of Technology and Economics, WIM VAN SAARLOOS, Leiden University, WOLFGANG LOSERT, University of Maryland College Park — Cooperative motion is a hallmark of dense granular media. Using the laser sheet scanning method described in [1], we are able to track the motions of all particles in a dense packing of spheres in three dimensions. We analyze the motions of all particles within a split bottom shear cell. We study both steady and oscillatory shearing processes. We compare relative motions of neighboring particles using a measure, \(P(\cos(\alpha))\), based on a measure originally used by Ellenbroek et al [1]. The angle, \(\alpha\), is the angle between the relative displacements of neighboring particles and their bond vectors. A pair of neighboring particles where \(\cos(\alpha)=0\) is called a rolling contact. We find that particles in contact tend to roll past one another, which is consistent with the findings made by Ellenbroek et al for systems close to jamming. We also find that the number of rolling contacts drops at the onset of a shear reversal. [1] Slotterback et al, to appear in Phys Rev Lett [2] Ellenboek et al., Phys Rev Lett, 97 258001 (2006).
Three-dimensional Order and Self-Diffusion in a Cyclically Sheared Granular System. ANDREAA PANAITESCU, ARSHAD KUDROLLI, Physics Department, Clark University — We investigate the structure and dynamics of a dense granular packing (consisting of one millimeter diameter spherical glass beads) undergoing cyclic shear obtained by smoothly deforming a parallelped shaped cell. Using a fluorescent refractive index matched particle tracking technique, we obtain the three dimensional position of particles in the central region of the shear cell as a function of shear cycle. The granular packing is observed to evolve towards crystallization over thousands of shear cycles and the packing fraction is correspondingly observed to increase smoothly from loose packing fraction. We obtain the Voronoi cell volume distributions from the measured positions, and compare them with various models which predict a Gamma-distribution and help us define a regularity factor. Further, we discuss the measured radial distribution and the bond-order parameter Q6 which are widely used to quantify local order in spherical particle systems. We find that the initial self-diffusion of the particles is anisotropic with diffusion greater in the flow direction compared with the velocity gradient direction which in turn is greater than the vorticity direction.

1:03PM W14.00010 Dynamic effective mass of granular media. DAVID JOHNSON, Schlumberger-Doll Research, ROHIT INGLE, JOHN VALENZA, CHÃœUR-JIAN HSU, NICOLAS GLAND, HERMAN MAKSE, SCHLUMBERGER-DOLL RESEARCH COLLABORATION, LEVICH INST. COLLABORATION — We report an experimental and theoretical investigation of the frequency-dependent effective mass, \( M(\omega) \), of loose granular particles which occupy a rigid cavity to a filling of 48%, the remaining volume being air of differing humidities. We demonstrate that this is a sensitive and direct way to measure the properties of the granular medium that are the cause of the changes in acoustical properties of structures containing grain-filled cavities. Specifically, we apply this understanding to the case of the flexural resonances of a rectangular bar with a grain-filled cavity within it. The dominant features of \( M(\omega) \) are a sharp resonance and a broad background, which we analyze within the context of simple models. We find that: a) These systems may be understood in terms of a height-dependent and diameter-dependent effective sound speed (\( \sim 130 \text{ m/s} \)) and an effective viscosity (\( \sim 2 \times 10^4 \text{ Poise} \)). b) There is a dynamic Janssen effect in the sense that, at any frequency, and depending on the method of sample preparation, approximately one-half of the effective mass is borne by the side walls of the cavity and one-half by the bottom. c) On a fundamental level, dissipation is dominated by adsorbed films of water at grain-grain contacts in our experiments.

1:15PM W14.00011 ABSTRACT WITHDRAWN –

1:27PM W14.00012 Visualization of displacement fields in sheared granular systems. KINGA LORINCZ, PETER SCHALL, University of Amsterdam — The jamming transition, i.e. the transition in a granular system from rest to flow is a fundamental problem of great importance to the understanding of a wide class of disordered materials: grains, clay and glassy materials such as molecular glasses and gels. We visualize the particles in a sheared three-dimensional granular packing immersed in an index matching liquid using confocal microscopy and laser sheet imaging. These experimental methods allow for an accurate determination of the displacement field of the particles at the onset of flow.


11:15AM W15.00001 Assembly and melting of DNA nanotubes and tile lattices. THOMAS SOBEY, STEPHAN RENNER, FRIEDRICH SIMMEL, Biomolecular Systems und Bioelectronics, Physics Department E14, Technical University Munich, 85748 Garching, Germany — Programmable molecular self-assembly using DNA is allowing the demonstration of increasingly novel nanoscale structures such as lattices and tubes. Understanding the assembly and melting pathways of these will allow us to develop more complex and/or stable structures, and potentially useful nanomaterials. We experimentally show differences in these pathways by correlating temperature-controlled UV absorption measurements with atomic force microscopy, fluorescence microscopy, and transmission electron microscopy measurements. The three-dimensional nanotubes assemble in several hierarchical steps but melt in a single step, and this contrast is proposed to arise from the fundamental distinction between three-dimensional closed tubes and two-dimensional open lattices.

11:27AM W15.00002 Response of a self-assembling to mechanical stress\(^1\). YVES DUBIEF, University of Vermont, Mechanical Engineering and Material Science Program, ROSS PACKARD, University of Vermont, Material Science program, SREEDHAR MANCHU, LEONIE COWLEY, University of Vermont, Mechanical Engineering Program — Coarse-grained molecular dynamics is used to characterize the mechanical properties of a solution of phospholipids and polyelectrolytes under shear and compression. DPPC (1,2-Dipalmitoylphosphatidylcholine), polyelectrolytes and water are coarse-grained using the MARTINI force field. Simulations are performed using both GROMACS and LAMMPS. In our simulation, the solution is confined by two parallel walls, with the objective of this study being (i) to study the influence of the electrostatic nature of the wall on the self-assembling structure of the solution and (ii) to define the rheological and structural response of the solution under shear and compression by moving one wall.

\(^1\)The computational support of the Vermont Advanced Computing Center is gratefully acknowledged. Y. Dubief and S. Manchu also thank Vermont Epscor and NSF for their support.

11:39AM W15.00003 Self-assembling structures resulting from the presence of polyelectrolytes in a solution of phospholipids\(^1\). ROSS PACKARD, YVES DUBIEF. University of Vermont — The objective of this study is the characterization of self-assembled structures formed by the combination of phospholipids and polyelectrolytes. Coarse-grained molecular dynamics is used to simulate solutions of DPPC (1,2-Dipalmitoylphosphatidylcholine) and polyelectrolytes in three dimensional periodic domain. The MARTINI database defines the topology of coarse-grained macromolecules and water and simulations are performed using GROMACS. The interaction between negatively charged polyelectrolytes and positively charged hydrophilic heads of DPPC causes the disruption of lipid bilayer membranes and vesicles. The study attempts to define the conditions necessary for the formation of vesicles or organized networks of lipid bilayers that encapsulate the polyelectrolytes. Such structures are suspected to play an important role in biological fluids subject to large mechanical stress.

\(^1\)The computational support of the Vermont Advanced Computing Center is gratefully acknowledged.

11:51AM W15.00004 Self-organized Gels in DNA/F-Actin mixtures without Crosslinkers. JOHN BUTLER, GHEE HWEE LAI, OLENA ZRIBI, University of Illinois at Urbana-Champaign, IVAN SMALYUKH, University of Colorado at Boulder, THOMAS ANGELINI, Havard University, KIRSTIN PURDY, University of Illinois at Urbana-Champaign, RAMIN GOLESTANIAN, University of Sheffield, GERARD C. L. WONG, University of Illinois at Urbana-Champaign — Interactions between flexible chains and rigid rods govern a broad range of soft matter systems. As a model system of like-charged rigid rods and flexible chains, we examine mixtures of DNA and filamentous actin (F-actin). Confocal microscopy reveals the formation of elongated nematic F-actin domains reticulated via defect-free vertices into a network embedded in a mesh of random DNA. Synchrotron small-angle x-ray scattering (SAXS) indicates that the DNA mesh squeezes the F-actin domains into a nematic state with an inter-actin spacing that decreases with increasing DNA concentration. Salt strongly influences the domain sizes and transitions the system from a counterion-controlled regime to a depletion-controlled regime, both mechanisms of which are entropic in origin.
12:03PM W15.00005 Modeling the hydrophobic effect by coupling solutes to a lattice gas . AMISH Patel, DAVID CHANDLER, University of California, Berkeley — In problems of biological assembly, manifestation of the hydrophobic effect is complex depending on the size as well as the conformation of the solute. The solute disrupts the inherent structure of the solvent by causing an unbalancing of attractive interactions experienced by the solvent molecules. The extent of this disruption determines the relative ease with which the solute is solvated. The theory of Lun, Chandler and Weeks (LCW) successfully describes this rich interplay between the solute and solvent structures by coarse-graining the solvent density and analytically integrating out solvent fluctuations on length-scales smaller than the coarse-graining length ($L_c$). Since the implementation of LCW theory can be computationally demanding, we have coarsened the coarse-grained solvent density was mapped onto a lattice gas by ten Wolde, Sun and Chandler. In this work, we further improve upon the theory by relaxing certain assumptions about the unbalancing of attractive interactions on length scales smaller than $L_c$. In addition to a brief overview of the theory, results obtained by application of the theory to several pertinent problems of biological assembly will be presented.

12:15PM W15.00006 Direct Measurement of Inter-filament Forces in Neurofilament Networks: Synchrotron X-ray Diffraction Study under Osmotic Pressure . R. BECK, J. DEEK, C.R. SAFINYA, UC Santa-Barbara — Neurofilaments (NFs) are the major protein constituents in neuronal processes (axons and dendrites) that impart mechanical stability and act as structural scaffolds. The filaments assemble from three different subunit proteins (NF-L, NF-M, NF-H) to form a 10 nm diameter flexible polymer with radiating unstructured sidearms. Recent work showed, that at high protein concentration, the NFs form a nematic hydrogel network with a well-defined interfilament spacing as can be measured by synchrotron small-angle x-ray scattering (SAXS) [1]. In order to directly elucidate the interfilament forces responsible for the mechanical properties of NFs hydrogel, we conducted a SAXS-osmotic pressure study, which yielded pressure-distance curves at different subunit compositions and monovalent salts. We show that filaments composed with NF-L and NF-M strongly attract each other through their polypeptide sidearms, in particular at high monovalent salt. However, filaments comprised of NF-L and NF-H show a distinctly different pressure-distance dependency, with much larger interfilament spacing and weaker salt dependence. Supported by DOE DE-FG-02-06ER46514, NIH GM-59288, NSF DMR-0805103, and the Human Frontier Science Program organization. [1] J.B. Jones, C.R. Safinya, Biophys. J. 95, 823 (2008)

12:27PM W15.00007 Flexible ferromagnetic filaments and the interface with biology: ANDREJS CEBERS, MIHAIJS BELOVS, KASPARS ERLGIS, University of Latvia — Flexible ferromagnetic filaments exist in Nature (magnetotactic bacteria use them for the navigation purposes in the magnetic field of the Earth) and may be synthesized artificially by linking the functionalized ferromagnetic particles by DNA fragments of definite length. Ferromagnetic filaments allow to mimic self-propulsion of microorganisms by using AC magnetic fields. It is investigated both theoretically and experimentally. The elastic properties of the filaments are studied by kinetics of their orientation in an AC magnetic field of enough high frequency and allow to observe the described behavior of the filaments at reversal of the magnetic field. By numerical analysis the Floquet coefficients for the dynamics of ferromagnetic filaments are calculated and the existence of stationary oscillations of U-like shapes is confirmed. These shapes self-propel perpendicularly to the AC magnetic field.

1:03PM W15.00010 Biomotor-functionalized Nanowires for Nanobio-mechanical Applications . DONG SHIN CHOI, NANO Systems Institute, Seoul National University, ALEXANDER PETROV, Institute of Solid State Physics, Bulgarian Academy of Sciences, ANTL JAKLI, Liquid Crystal Institute, Kent State Univ. — The effects of chirality of membrane-forming lipids, has been largely ignored at present. Here we demonstrate that the chirality of phospholipids makes fluid lipid bilayers piezoelectric. This implies that chiral lipids would play a central role in the functioning of cell membranes as active mechano-transducers. By periodically compressing nonaqueous lamellar phases of left (L-alpha-Phosphatidylcholine), right (D-alpha-Phosphatidylcholine) and racemic (DL-alpha-Phosphatidylcholine) lipids, we induced a tilt of the molecules with respect to the bilayer’s normal and produced an electric current perpendicular to the tilt plane with the chiral lipids but not with a racemic mixture. This effect occurs because the lipids from a SmA$^*$_phase liquid crystal structure of the bilayers. Under molecular tilt, a ferroelectric SmC$^*$ phase is formed, creating a polarization which is normal to the tilt plane. This coupling allows for a wide variety of sensory possibilities of cell membranes such as mechanooception, magneto-sensitivity, as well as in-plane proton membrane transport and related phenomena like ATP-synthesis, soft molecular machine performance, etc.

1:15PM W15.00011 Non-monotonic mobility vs. length dependence observed in electrophoretic separation of 25 bp DNA ladder in Pluronic gels . SEUNGYONG YOUNG, DAVID VAN WINKLE, Department of Physics and Center for Materials Research and Technology, Florida State University — We electrophoresed a double-stranded DNA ladder first in an agarose gel, then in gels of Pluronic F-127 at room temperature. The DNA ladder consisted of 19 discrete fragments ranging in length from 25 to 450 bp at 25 bp increments plus 500 bp. The DNA fragments were first separated in agarose gel and stacked normally with 25 bp having the highest mobility. A single lane of the separated DNA ladder in the agarose gel was inserted at the edge of a Pluronic gel slab. The DNA was electrophoresed from the agarose into the Pluronic gels perpendicular to the original separation axis. Mobilities of DNA fragments increased from 25 bp to 175 bp and then decreased from 175 bp to 500 bp. The 25 bp and 500 bp bands of the ladder had the same mobility in several different Pluronic gel concentrations. Both were slower than most bands in between. The highest mobility fragments with length of 175 bp have 59.5 nm contour length which is about 3.5 times the diameter of a micelle (17 nm). This result suggests a crossover from chromatographic separation to electrophoretic separation for these short DNA's. This research is supported by the state of Florida (Martech) and Research Corporation.
1:27PM W15.00012 Partition function and space-filling fractal-like networks of branching tubes. SAMIR LIPOVACA — We may think of the probability in quantum mechanics as a sort of fluid that flows from one point to another continuously and without loss or gain. We will utilize this fluid idea and imagine that probability flows through a space-filling fractal-like networks of branching tubes similar to the networks of a general model for the origin of allometric scaling laws in biology. In the general model, scaling laws arise from the interplay between physical and geometric constraints. This model provides a complete analysis of scaling relations for mammalian circulatory systems that are in agreement with data. We will show that there is a connection between a quantum system in thermal equilibrium and space-filling fractal-like networks. The relationship will be revealed through the calculation of the total fluid (probability) network volume. We will show that this total volume is proportional to the partition function of the related quantum system.

1:39PM W15.00013 The impact of conformational fluctuations on self-assembly: Cooperative aggregation of archaenal chaperon proteins, STEPHEN WHITEHALL, Lawrence Berkeley National Laboratory, CARL ROGERS, ANDREA PASQUA, UC Berkeley, CHAD PAAVOLA, JONATHAN TRENT, NASA Ames Research Center, PHILLIP GEISSLER, UC Berkeley — Protein complexes called rosettasomes self-assemble in solution to form large-scale filamentous and planar structures. The relative abundance of these aggregates varies abruptly with environmental conditions and sample composition. Our simulations of a model of patchy nanoparticles can reproduce this sharp crossover, but only if particles are allowed to switch between two internal states favoring different geometries of local binding. These results demonstrate how local conformational adaptivity can fundamentally influence the cooperativity of pattern-forming dynamics.

Thursday, March 19, 2009 2:30PM - 5:30PM — Session X14 DFD: Micro and Nano Fluid Mechanics 315

2:30PM X14.00001 The dynamical origin of the zeta potential. PATRICK TABELING, ESPCI — By using evanescent waves, we study equilibrium and dynamical properties of liquid-solid interfaces in the Debye layer for hydrophilic and hydrophobic surfaces. We measure velocity profiles and nanotracr concentration and diffusion profiles between 20 and 300 nm from the walls in pressure-driven and electroosmotic flows. We extract electrostatic and zeta potentials and determine hydrodynamic slip lengths with 10 nm accuracy. The spectacular amplification of the zeta potential resulting from hydrodynamic sliplappags allow to clarify for the first time the dynamic origin of this potential.

2:42PM X14.00002 Radiofrequency Nanoelectolytic Debye-Layer Transistor. JEAN-LUC FRAIKIN, UC Santa Barbara, MICHAEL REQUA, MICHAEL STANTON, ANDREW CLELAND, UC Santa Barbara — A voltage-biased metal immersed in an aqueous electrolyte attracts ions from the solution, causing the accumulation of a diffuse layer of charge close to its surface. This layer is called the Debye-Huckel layer, or double layer. For a non-reactive electrode, the electric double-layer (EDL) presents a capacitive electrical impedance, which depends non-linearly on the voltage applied across it. We present a novel transistor whose transduction element is the EDL capacitance, which allows electronic gating of a 50 MHz signal at frequencies close to 1 MHz. The transistor comprises three terminals: a pair of nanofabricated interdigitated electrodes (IDES) embedded in an electrolyte-filled microfluidic channel, and a third, gating Ag/AgCl electrode in the same fluid volume. We demonstrate direct gating of the transistor with the Debye layer, and make use of the device to measure the voltage dependence of the EDL capacitance over a broad range of electrode bias.

2:54PM X14.00003 Simulation of Steady-State Non-Equilibrium Ion Distributions Within a Finite-length Nanofluidic Channel. WILLIAM BOOTH, JARROD SCHIFFBAUER, JOSH FERNANDEZ, KATHLEEN KELLEY, AARON TIMPERMAN, BOYD EDWARDS, West Virginia University, EDWARDS MICROFLUIDICS RESEARCH GROUP TEAM, TIMPERMAN’S ANALYTICAL CHEMISTRY GROUP TEAM — Steady-state non-equilibrium distributions of two species of mono-valent ions near and within a charged 2D nanofluidic channel have been examined with and without electroosmotic flow. Large reservoirs are connected by the nanofluidic channel to simulate bulk conditions. Far-from-equilibrium applied voltages create a charge polarization across the nanochannel when the Debye length is comparable to the channel width. Depletion zones of each ion species are observed.

3:06PM X14.00004 DEP Force Spectroscopy. JINGYU WANG, STEVEN M.T. WEI, JOSEPH JUNIO, H.D. OU-YANG, Lehigh University — We report measurement of the frequency-dependent dielectrophoretic forces imparted on individual colloidal particles in an aqueous suspension. The motion of suspended particles relative to the solvent resulting from polarization forces due to an inhomogeneous electric field is known as the dielectrophoretic force (DEP). In the case of colloidal particles, the Clausius-Mossotti (CM) function containing the frequency dependence of the dielectric behavior of the particle relative to the suspending fluid dictates the direction and magnitude of the resulting DEP force. The magnitude of this force approaches zero as the frequency approaches the point of cross-over to switch the direction of the force. Using optical tweezers as force sensor we have successfully characterized the frequency dependent DEP force with a spatial resolution in the micron range and a force resolution of a fraction of 1 pN. To achieve this, we used an AM modulation scheme to administer the oscillating electric field, so that we could monitor the phase and amplitude of the displacement of the particle while it was held by the optical tweezers and acted on by the DEP force. The optical tweezers based DEP force spectroscopy presents a way to understand the fundamental parameters at the microscopic level.

3:18PM X14.00005 A New Fourier Model of Traveling Wave Electrophoresis. ROBERT CORRELL, JAMES EAKINS, West Virginia University, JAMES VOPAL, West Liberty State College, BOYD EDWARDS, West Virginia University — Traveling-wave electrophoresis is a new method of separating charged analytes using a series of interlaced electrodes with time-varying electric potentials along a microchannel. It potentially offers several potential advantages over conventional electrophoretic devices, including increased separation efficiency and ease of scalability. A better description of the underlying mathematics is required in order to fully optimize this promising technology. As such, a new Fourier model of the electric potential inside the channel is introduced, along with preliminary computational results. This new representation allows for greatly reduced computation time and greater accuracy. Similarities and differences with other models are highlighted, as well as the dependence of the potential on the electrode and channel geometries. The movement of charged particles in response to the potential is examined, with several critical thresholds highlighted.

3:30PM X14.00006 Traveling-wave electrophoresis for microfluidic separations, BOYD EDWARDS, West Virginia University, AARON TIMPERMAN, LLOYD CARROLL, KYOO JO, JON MEASE, JARROD SCHIFFBAUER — Models and microfluidic experiments are presented of an electrophoretic separation technique in which charged particles whose mobilities exceed a tunable threshold are trapped between the crests of a longitudinal electric wave traveling through a stationary viscous fluid. The wave is created by applying periodic potentials to electrode arrays above and below a microchannel. Predicted average velocities agree with experiments and feature chaotic attractors for intermediate mobilities.

We acknowledge funding from the US Department of Energy and BioSim European Union Network of Excellence.

1We acknowledge funding from NSF grants DMR-0647763 and EPS-0554328, and a WVU Research Corporation grant.

1Funding from NSF grants DMR-0647763 and EPS-0554328, and a WVU Research Corporation grant.
3:42PM X14.00007 Trigonometric Model for Traveling Wave Electrophoresis, JAMES VOPAL, West Virginia University./West Liberty State College, BOYD EDWARDS, West Virginia University. The motion of ions in a trigonometric spatio-temporal potential in a fluidic microchannel is investigated. Computer simulations are performed for ions of different mobilities to predict the ion trajectories and average velocities. In many instances, plotting the average velocity versus mobility results in a Devil’s staircase. When Devil’s staircases are seen, no chaotic behavior is present. When the average velocity versus mobility does not result in a Devil’s staircase, chaotic trajectories can be found.

3:54PM X14.00008 Electokinetic interaction between a charged cylindrical particle and a charged planar surface, YONG KWEON SUH1, KANG SANGMO, KANG YONG, VIJAY FERNANDEZ DOLFRED, SUH YONG KWEON, Department of Mechanical Engineering, Dong-A University, Busan, 604714. Electrokinetic motion of a charged particle under an electric field applied parallel to the planar surface has been studied numerically. Effect of electric double layer (EDL) interaction between the particle and the surface on the electrophoretic motion is the main focus of the study. Thick EDL around the particle and on the surface is obtained by solving Poisson-Nernst-Planck (PNP) equations on a hybrid grid system. A Lagrange type cylindrical grid attached to the particle can move freely on Euler type Cartesian grid. Second order accurate bilinear-interpolation scheme is used at the intersection of Lagrange-Euler grid. The linear and rotational motion of particle in the electroosmotically driven fluid is obtain by balancing EDL interaction force, gravitational force, and hydrodynamic force. The fluid flow along the surface and around the particle is computed by solving Stokes equations.

4:06PM X14.00009 Ac electroosmotic flows above coplanar electrodes, YONG KWEON SUH, Department of Mechanical Engineering, Dong-A University. Interactive numerical method has been proposed to calculate the ac electroosmotic flows above a pair of coplanar electrodes. The thin electrical triple layer (ETL) has been modeled by an asymptotic theory developed by the authors. The model corresponds to a simple dynamic equation for the surface charge density representing the integrated charge over the inner layer. Interactive calculation of the dynamic equation and the Laplace equation for several periods of ac frequency then yielded steady-state distribution of potential and the potential drop across the Stern and inner layers. The Smoluchowski’s slip velocity was then determined from those two set of data and used as the boundary condition for the calculation of the Stokes flow above the electrodes. We have shown that our solutions compared well with the experimental data reported in the literature. We investigated the effect of various parameters on the slip velocity distribution, such as the ac frequency, the electrode length, the effective Stern-layer thickness and the adsorption coefficients.

4:18PM X14.00010 Detection and electrokinetic trapping of single fluorescent molecules in fused silica nanochannels, BRIAN CANFIELD, XIAOXUAN LI, WILLIAM HOFMEISTER, LLOYD M. DAVIS, University of Tennessee Space Institute. We describe experimental detection and electrokinetic trapping of single, fluorescently-labeled proteins confined within ~100 nm fluidic channels fabricated in fused silica. Though difficult to fabricate, the fused silica environment yields lower autofluorescence than borosilicate glass, which is especially advantageous given the low light level from single molecules. The molecules are dispersed in a buffer solution at ultralow concentration (~10^11-12 M) to probe single-molecule occupancy of the sub-femtoliter probe volume within the nanochannel. Fluorescence is excited and collected in a custom-built confocal microscope, using two temporally interleaved beams from a modelocked dye laser focused to adjacent spots along the nanochannel. Detection is accomplished with custom single-photon avalanche diodes for time-resolved single-photon counting, and by using this time stamp information, a field-programmable gate array circuit board controls the electrokinetic trapping by modulating an applied voltage. Fluorescence correlation spectroscopy is also used to monitor the transport of molecules along the nanochannel. Electrophoretic transport can thus be characterized from changes in the autocorrelation function with voltage modulation.

4:30PM X14.00011 Microfluidic device for the electrokinetic manipulation of single molecules, JASON KING, LLOYD DAVIS, BRIAN CANFIELD, WILLIAM HOFMEISTER, University of Tennessee Space Institute, PHILIP SAMPSON, Vanderbilt University. We are developing a microfluidic device for the electrokinetic manipulation of single fluorescent molecules in solution. A device consists of electrode pairs deposited onto glass cover slips via UV microlithography and ion sputtering. By positioning two such electrode pairs in a tetrahedral configuration separated by 100 microns and applying appropriate digitally-controlled voltages to each, the apparatus generates an electric field of selected directionality in the central bounded region. Proof of concept is demonstrated by controlling the motion of micron-size latex beads, visualized with an EM-CCD microscope. When 40 kHz-Sapphire laser pulses (repetition rate 76 MHz) are split into four temporally interleaved pulses (effective rate 304 MHz), which are then focused to the vertices of a tetrahedron (approximately one micron per side) within the central electrode region to generate two-photon-excited fluorescence from single molecules. The time stamp data from this four-focus probe, collected with a custom fast-timing single-photon avalanche diode, enables characterization of particle motion through fluorescence cross-correlation spectroscopy.

4:42PM X14.00012 Microfluidic Channels under Magnetohydrodynamic (MHD) Convection, YOGENDRA M. PANTA, HYUN W. KIM, Department of Mechanical Engineering, Dong-A University, Busan, 604714. Electrophoretic motion of a charged particle under an electric field applied parallel to a planar surface has been studied. The motion of ions in a trigonometric spatio-temporal potential in a fluidic microchannel is investigated. Computer simulations are performed for ions of different mobilities to predict the ion trajectories and average velocities. In many instances, plotting the average velocity versus mobility results in a Devil’s staircase. When Devil’s staircases are seen, no chaotic behavior is present. When the average velocity versus mobility does not result in a Devil’s staircase, chaotic trajectories can be found.

4:54PM X14.00013 Cell and Colloidal Substrates for Dielectrophoretic Microfluidic Immunoassays, JILL MAZUR, ZACHARY GAGNON, HSUEH-CHIA CHANG, University of Notre Dame, Department of Chemical and Biomolecular Engineering. Dielectrophoresis (DEP) is a term commonly used to describe the field induced polarization and translational motion of a polarizable particle in a non-uniform AC field. The frequency at which the induced particle dipole goes to zero, known as the crossover frequency (cof), is highly dependent on the surface conductance of the particle. We have shown previously that DNA hybridization on the surface of a 100 nm functionalized silica particle leads to detectable surface conduction changes which make it possible to detect DNA hybridization reactions by simply measuring changes in particle suspension cof. In this work we present a similar detection scheme using novel colloidal and cell substrates as dielectrophoretic immunosensors. Aminated cell or nanocolloid surfaces are subjected to a polymer coating glutaraldehyde treatment followed by antibody coupling reaction for immunoassay based detection. By varying the polymer coating thickness on the colloidal or cell surface we demonstrate the ability to tune, stabilize the cell and colloid cof, and minimized non-specific adsorption of proteins. As such, a library of cof labeled colloids and cells are created and used for multiple antigen analysis. By measuring the colloid and cell specific DEP cof prior to and after antibody-antigen interaction we demonstrate the ability to perform rapid label free protein detection within a microfluidic device.
This approach provides facile route to analyze fluctuation dynamics in liquid crystals. The elastic constant to the viscosity ratio was computed from the relaxation frequency estimated from the relaxation dynamics. The twinkling of liquid crystals due to orientational fluctuations are sufficiently slow and large, have long wavelength and increase with temperature. Herein, we describe our study on fluctuation dynamics by high speed imaging. Liquid crystals usually have fluctuations with respect to their director, even when the molecular axes tend to be aligned to each other. These fluctuations are fast and determined by the line tensions of the islands and by the film’s viscosity. Then the region that used to be the thicker island expands and eventually covers the whole merged island. This process which is dependent on the permeation between layers in addition to the line tension and viscosity, is much slower. The shapes of the islands are extracted from high speed camera images and compared with model calculations.

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

2:30PM X15.00001 The Taming of the Screw: Nonlinear Interactions in Smectic Liquid Crystals & SENSORS, ELISABETTA MATSUMOTO, GARETH ALEXANDER, RANDALL KAMien, University of Pennsylvania — From the twist grain boundary phase to the smectic phases of bent core liquid crystals, beautiful and intricate textures composed of screw dislocations appear time and again in a wide variety of smectic systems; yet, little is known about the interactions of screw dislocations. The linear smectic free energy is not sufficient to describe the energetics of single screw dislocations, and superposition cannot shed light on the interaction of many such defects. The full rotationally invariant nonlinear smectic free energy provides insight into systems of multiple screw dislocations. Such nonlinear interactions allow us to begin to understand the stability of the bulk phases observed in both smectic A liquid crystals and their chiral smectic C* counterparts.

2:42PM X15.00002 Coalescence Dynamics Analysis Of Islands In Smectic A Freely Suspended Films1, ZOOM NGUYEN, University of Colorado, Boulder, CHEOL PARK, JOSEPH MACLENNAN, MATTHEW GLASER, NOEL CLARK — We explore the coalescence dynamics of circular islands in smectic A freely suspended liquid crystal films. The process typically has two distinct stages. First, when the islands make contact initially, the thinner island wraps around the thicker one. These dynamics are fast and determined by the line tensions of the islands and by the film’s viscosity. Then the region that used to be the thicker island expands and eventually covers the whole merged island. This process which is dependent on the permutation between layers in addition to the line tension and viscosity, is much slower. The shapes of the islands are extracted from high speed camera images and compared with model calculations.

3:06PM X15.00003 Modeling twisted distortions in nematic elastomers1, VIAMNEY GIMENEZ, BADEL MBANGA, FANGFU YE, JONATHAN SELINGER, ROBIN SELINGER, Liquid Crystal Institute, Kent State Univ. — Experimental studies have reported that nematic elastomers with a twisted nematic director—similar to the configuration in a twisted nematic cell—show a well-controlled deformation under change of temperature. Due to the difference in thermal expansion along and perpendicular to the nematic director, the sample twists and curls dramatically under heating and cooling [1]. We model this shape evolution using both analytical calculations and finite element elastodynamics simulations. In analytical calculations, we determine the optimal shape of an initially flat strip by minimizing a free energy functional that takes into account the coupling between orientational order and mechanical strain. We compare which of two final states—a helical or twisted ribbon shape—is lower in free energy, as a function of the sample’s aspect ratio and material properties. We then use finite element simulations to model the dynamics of this spontaneous deformation and examine the resulting equilibrium shapes, which may be intermediate between helical and twisted. Results are compared to relevant experiments. We also use our simulation model to explore a wider variety of director configurations and sample geometries, beyond the ideal cases solvable via analytical methods. [1] G. Mol, K. D. Harris, C. W. M. Bastiaansen, and D. J. Broer, Adv. Funct Mater, 15, 1195 (2005).

1 All of Dr. Mohan Srinivasarao’s school and center is at Georgia Institute of Technology

5:06PM X14.00014 AC Electrokinetic Cell Separation on a Microfluidic Device, ZACHARY GAGNON, University of Notre Dame, Dept. Chemical and Biomolecular Engineering, HSUEH-CHIA CHANG, University of Notre Dame, Department of Chemical and Biomolecular Engineering — Rapid cell separation and collection is demonstrated through the integration of electrokinetic pumps, dielectrophoretic (DEP) traps and field driven valves into a well designed microfluidic channel loop. We present the ground-up design and analysis of this fully functional microfluidic device for the rapid separation and collection of live and dead yeast cells and malaria red blood cells (RBCs) at low concentrations. DEP cell sorting and concentration schemes are based on the exploitation of cell specific DEP crossover frequencies (cof’s). A rigorous DEP study of yeast and RBCs is presented and used to determine optimal conditions for cell separation. By utilizing a glutaraldehyde crosslinking cell fixation reaction that is sensitive to cell membrane protein concentration, we demonstrate the ability to further amplify these differences between healthy and unhealthy cells as well as stabilize their DEP cof’s. Pumping is achieved with a new type of electrokinetic flow, AC electrothermal electro-osmosis (ETEO) and is shown to scale inversely with the field induced debye length and drive fluid velocities in excess of 6 mm/sec. The well characterized electrokinetic phenomena are integrated into a microchannel loop with a specifically designed electrode field penetration length for low concentration cell separation and concentration.

5:18PM X14.00015 Anomalous analyte dispersion at microchannel-nanopipillary membrane interfaces, JARROD SCHIFFBAUER, Physics Dept, West Virginia University, KATHLEEN KELLY, Chemistry Dept , West Virginia University, WILL BOOTH, Physics Dept., West Virginia University, JOSH FERNANDEZ, Chemical Engineering, Dept., West Virginia University, AARON TIMPERMAN, Chemistry Dept., West Virginia University, BOYD EDWARDS, Physics Dept. West Virginia University — The dispersion of a plug-like distribution of negatively charged fluorescent dye molecules inside a microchannel is studied by numerical analysis of a time-series of epifluorescence microscope images. The concentration is accomplished using a nanopipillary membrane (NCM) –based concentration device. Dispersion of the analyte after concentration is complete, i.e. after the applied voltage is removed, is of considerable technical interest as a limiting factor in the functionality of lab-on-a-chip concentration devices. Subsequent band-broadening is inconsistent with Taylor dispersion and is shown here to be influenced by the presence of charge-separation between the concentrated analyte and background buffer ions.
3:18PM X15.00005 Behavior of Focal Conic Defects in Shear Flow, SOURAV CHATTERJEE, SHELLEY ANNA, Carnegie Mellon University — The rheology of layered liquids is influenced to a large extent by defects present in the system, especially in small gaps. Toroidal focal conic defects are a common type of defect in small molecule layered liquids. We present a study of the influence of flow on focal conic defects in smectic liquid crystals, generated by antagonistic boundary condition at the surfaces. The defects are confined in gaps of the order of tens of microns and are subject to simple shear. The sizes of the focal conic defects vary with the gap size, and hence visual observations are made as to how the gap influences the dynamics of the focal conic defects in a shear flow. We also observe instabilities in initially defect free samples that lead to the creation of defects. The results offer insight into the complex relationship between defects and flow.

3:30PM X15.00006 Polarization current as evidence of local anticlinic correlations in de Vries smectics, Z. V. SMITH, P. D. BEALE, R.-F. SHAO, L. WANG, D. M. WALBA, N. A. CLARK, M. A. GLASER, LCMRC, U. of Colorado, Boulder — Previous theoretical work on the electrochemical response of chiral de Vries SmA materials based on the electric field-induced reorientation of independent tilt domains [J. V. Selinger et al., Phys. Rev. E 64, 061705 (2001)] fails to account for the sigmoidal dependence of induced polarization (P) on field (E) seen in some materials. To account for this behavior, we model de Vries smectics as ensembles of small but finite anticlinic tilt domains. Within each domain, interlayer tilt coupling favors anticlinic interfaces, but the finite range of in-layer tilt correlations leads to thermally activated synclinic interfaces and a finite tilt correlation length along the layer normal. This model, equivalent to a generalized one-dimensional XY model in an external field with quadratic and quartic nearest-neighbor interactions, is studied by Monte Carlo simulation and transfer matrix methods. The model successfully reproduces the dependence of P on E for a specific material (W530), and yields physical parameters such as the in-layer correlation length and effective interlayer tilt coupling. The predicted anticlinic tilt correlations should be observable as diffuse superlattice reflections in polarized resonant x-ray scattering experiments.

3:42PM X15.00007 A one order parameter tensor description of biaxial nematic liquid crystals, XIAOYU ZHENG, Department of Mathematical Sciences, Kent State University, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University — We present a simple one order parameter tensor mean field theory of biaxial nematic liquid crystals. We construct the free energy from molecular interactions, identify the components of the order parameter tensors, and obtain self-consistent equations, which are then solved numerically. The phase behavior is described via a 3D phase diagram. We discuss the connection between molecular properties and the coefficients in the Landau expansion.

3:54PM X15.00008 Elasticities and viscosities of a lyotropic chromonic nematic liquid crystal, KRISHNA NEUPANE, Kent State University, YURI NASTISHIN, Institute of Physical Optics, Lviv, Ukraine, ALAN BALDWIN, OLEG LAVRENTOVICH, SAMUEL SPRUNT, Kent State University — We have performed dynamic light scattering studies of the elastic moduli and viscosity coefficients in a uniformly aligned sample of a lyotropic chromonic nematic formed by 14 wt. % water solution of Disodium Cromoglycate [1]. These parameters show a significant anisotropy. In particular, the bend and splay moduli $K_{33}$ and $K_{11}$ are an order of magnitude higher than the twist modulus $K_{22}$, and the ratio $K_{33}/K_{11}$ shows an anomalous increase in temperature, which we attribute to the shortening of the aggregates. The bend viscosity is three orders of magnitude smaller than the splay and twist viscosities; all viscosity coefficients exhibit a strong temperature dependence.

4:06PM X15.00009 Reflection and transmission coefficients of a cholesteric liquid crystal film with a negative dielectric coefficient, SABRINA RELAIX, WENYI CAO, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University — A cholesteric liquid crystal (CLC) is a periodic dielectric structure where simple analytic solutions of Maxwell’s equations exist: light propagating along the helical axis has been first described by Mauguin in 1911 [1], for wavelengths much smaller than the helical pitch, and was formulated more generally by de Vries in 1951 [2]. The analytical solutions are for bulk CLCs and do not describe the optical properties of a finite thickness CLC film. Recently, analytic expressions for the reflection and transmission coefficients of a CLC slab have been obtained by solving Maxwell’s equations and satisfying boundary conditions [3,4], providing results for thick slabs which go beyond the limitation of numerical methods. We discuss how these results are modified when one of the dielectric coefficients is negative. We explore the connection with hyperbolic dispersion and negative index materials. [1] C. Mauguin, Bull. Soc. Fr. Miner. Cristallogr. 34, 6 (1911) [2] H. de Vries, Acta Crystallogr. 4, 219 (1951) [3] W. Cao, Ph.D. dissertation, Chemical Physics, Kent State University (2005) (http://e-LC.org) [4] S. Relaix, W. Cao and P. Palffy-Muhoray, to be published.

4:18PM X15.00010 Maier-Saupe Theory of Nematics in 4D, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University, XIAOYU ZHENG, Department of Mathematical Sciences, Kent State University — We extend the Maier-Saupe theory of nematics to 4 dimensions. We consider the interaction of cylindrically symmetric particles, and derive an effective single particle potential. Using this, we obtain the free energy and the self-consistent equation for the order parameter — a second rank traceless tensor. In 4D, the order parameter has three independent eigenvalues. We solve the self-consistent equation, and study the solutions as function of temperature. Our results give insight into the relation between orientational order parameters in different dimensions.

4:30PM X15.00011 Statistical mechanics of the flexoelectric effect in nematic liquid crystals, SUBHAS DHAKAL, JONATHAN V. SELINGER, Kent State University — Flexoelectricity is the phenomenon in which polarization is induced by imposed deformations of the director field in nematic liquid crystals. Recent experiments [1,2] have found that the flexoelectric effect is three orders of magnitude greater for bent-core liquid crystals than for conventional rod-like liquid crystals. To understand this experimental result, we develop a lattice model for the statistical mechanics of the flexoelectric effect. We perform Monte Carlo simulations and mean-field calculations to find the behavior as a function of interaction parameters, temperature, and applied electric field. The resulting phase diagram has four phases: isotropic, uniaxial nematic, biaxial nematic, and polar. In the uniaxial and biaxial nematic phases, there is a large splay or bend flexoelectric effect, which diverges as the system approaches the nematic-polar transition. This model may explain the large bend flexoelectric coefficient observed in bent-core liquid crystals, which have a tendency toward polar order. [1] J. Harden, B. Mbanga, N. Eber, K. Fodor-Csorba, S. Sprunt, J. T. Gleeson, and A. Jakli, Phys. Rev. Lett. 97, 157802 (2006). [2] J. Harden, R. Teeling, J. T. Gleeson, S. Sprunt, and A. Jakli, Phys. Rev. E 78, 031702 (2008).

1Work supported by NSF MRSEC Grant DMR-0820579.

4:42PM X15.00012 Reflection and transmission coefficients of a cholesteric liquid crystal film with a negative dielectric coefficient, SABRINA RELAIX, WENYI CAO, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University — A cholesteric liquid crystal (CLC) is a periodic dielectric structure where simple analytic solutions of Maxwell’s equations exist: light propagating along the helical axis has been first described by Mauguin in 1911 [1], for wavelengths much smaller than the helical pitch, and was formulated more generally by de Vries in 1951 [2]. The analytical solutions are for bulk CLCs and do not describe the optical properties of a finite thickness CLC film. Recently, analytic expressions for the reflection and transmission coefficients of a CLC slab have been obtained by solving Maxwell’s equations and satisfying boundary conditions [3,4], providing results for thick slabs which go beyond the limitation of numerical methods. We discuss how these results are modified when one of the dielectric coefficients is negative. We explore the connection with hyperbolic dispersion and negative index materials. [1] C. Mauguin, Bull. Soc. Fr. Miner. Cristallogr. 34, 6 (1911) [2] H. de Vries, Acta Crystallogr. 4, 219 (1951) [3] W. Cao, Ph.D. dissertation, Chemical Physics, Kent State University (2005) (http://e-LC.org) [4] S. Relaix, W. Cao and P. Palffy-Muhoray, to be published.

1This work was supported by the AFOSR under MURI grant FA9550-06-1-0337.

1This work was supported by the AFOSR under MURI grant FA9550-06-1-0337.

Work supported by NSF Grant DMR-0605889.
4:42PM X15.00012 Aggregates in Chromonic Liquid Crystal Phases of Aqueous Solutions of Sunset Yellow* , LEELA JOSHI, SHIN-WOONG KANG, DENA MAE AGRA-KOOIJMAN, SATYENDRA KUMAR, Department of Physics, Kent State University — Molecules of dye Sunset Yellow consist of flat poly-aromatic core and hydrophilic groups at the periphery. In aqueous environments, they self-organize into columnar aggregates mainly via $\pi-\pi$ interactions between aromatic cores. At high concentrations, dye aggregates develop orientational and positional orders to form the nematic (N) and columnar (C) mesophases. Synchrotron x-ray scattering and optical polarizing microscopy were used to better understand the growth of aggregates and mesophase formation. Average column height and their spatial organization strongly depend on concentration, temperature, and pH value of the solution. The aggregate size decreases with temperature exhibiting an Arrhenius behavior with mesophase dependent activation energy. A dramatic decrease in the aggregate size upon addition of HCl highlights their sensitivity to electrostatic interactions. *Work supported by grant NSF/DMR-086991.

4:54PM X15.00013 Aggregation Properties of the Chromonic Liquid Crystal Benzopurpurin 4B , CHRISTOPHER MCKITTERICK, PETER COLLINGS, Swarthmore College — Benzopurpurin 4B (BPP) is a textile dye very similar to the common indicator Congo Red. As is true for all chroomics, the absorption spectrum is concentration dependent at low concentrations. If this dependence is used to estimate a free energy change for aggregation, it is higher than has been determined for other systems. Unlike other recently investigated chromonic liquid crystals, BPP forms a liquid crystal phase at extremely low concentrations, about 0.5 wt%. Also, unlike these other chromonic liquid crystals, the aggregation kinetics are exceedingly slow. X-ray diffraction and light scattering measurements indicate that the aggregates of BPP are much larger than for chromonic systems that form liquid crystals at higher concentrations. BPP aggregates can be imaged using confocal microscopy, revealing a length distribution centered at 3 $\mu$m for a solution forced through a 0.2 $\mu$m filter. Over days the aggregates lengthen to well over 10 $\mu$m. The diameter of the aggregate images is slightly greater than the diffraction limit of the microscope, placing an upper limit on the diameter of 0.14 $\mu$m. These dimensions are consistent with the light scattering results.

5:06PM X15.00014 Generalized Nematohydrodynamic Boundary Conditions with Application to Bistable Twisted Nematic Liquid Crystal Displays1 , ANGBO FANG, Department of Physics, Hong Kong University of Science and Technology, TIEZHENG QIAN, Department of Mathematics, Hong Kong University of Science and Technology, PING SHENG, Department of Physics and the Institute of Nano Science and Technology, Hong Kong University of Science and Technology — Parallel to the highly successful Ericksen-Leslie hydrodynamic theory for the bulk behavior of nematic liquid crystals (NLC), we derive a set of coupled hydrodynamic boundary conditions to describe the NLC dynamics near NLC-solid interfaces. In our boundary conditions, translational flux (flow slippage) and rotational flux (surface director relaxation) are coupled according to the Onsager variational principle of least energy dissipation. The application of our boundary conditions to the truly bistable $\pi$-twist NLC cell reveals that the thus far overlooked translation-rotation dissipative coupling at solid surfaces can accelerate surface director relaxation and enhance the flow rate. This can be utilized to improve the performance of electro-optical nematic devices by lowering the required switching voltages and reducing the switching times.  

1A. Fang acknowledges support from the KAUST Global Research Partnership.

5:18PM X15.00015 Soft Micro- to Nanolithography Using Highly Periodic Smectic Liquid Crystal Defects , HEE-TAE JUNG, YUN HO KIM, Korea Advanced Institute of Science and Technology, DONG KI YOON, Samsung Electronics, HYEON SU JEONG, Korea Advanced Institute of Science and Technology, ORGANIC OPTO-ELECTRONIC MATERIALS LAB. TEAM — Achieving perfect long-range order with soft building blocks at high speed and high resolution is one of the most exciting interdisciplinary research areas in current materials science and nano-biotechnology. Here, we have developed highly periodic patterns with sub-micrometer features over large-areas using toric focal conic domains (TFCDs) originated from smectic liquid crystal (LC). TFCDs are accomplished by precisely controlling the surface and interfacial properties of smectic LC. In order to apply the smectic liquid crystal defect arrays in lithography, the hexagonal arrays of domain patterns are used as molds for ultraviolet (UV) curable polymers, thereby providing LC defect stamps with high spatial resolution over large areas. Our method was further utilized to transfer patterns with sub-micrometer features from the polymer stamp surface to a secondary surface by microcontact printing ($\mu$-CP). The patterning method based on LC defects has significant advantages over existing lithographic approaches: 1) the masters and stamps are easy to fabricate, 2) the masters and stamps provide long-range surface ordering over large-areas, 3) the periodic arrays are formed quickly in several seconds, and 4) the stamps can generate feature sizes on the micrometer and submicrometer length scales, and 5) the methodology offers the possibility of controlling the array geometry by altering the geometry of the confining channels.

Friday, March 20, 2009 8:00AM - 9:48AM — Session Y14 DFD: Nonequilibrium and Templated Assembly 315

8:00AM Y14.00001 Speeding up the understanding of Vertical Deposition of Diluted Colloids1 , WENCESLAO GONZÁLEZ-VIÑAS, MAXIMILIANO GIULIANI2, MOORTHI PICHUMANI3, University of Navarra — We measured the speed of contact line in vertical deposition of diluted micron sized polymeric colloids. We correlated these results with the obtained morphologies for the deposits. We show that low velocities correspond to the formation of monolayer and high velocities to multilayer. These new results are explained in terms of the local concentration of particles in the suspension near the contact line and the porosity of the pre-deposited structure. The effect of an applied electric field to the system is also reported.

1Partially supported by Departamento de Educación (Gobierno de Navarra) 
2Supported by the Asociación de Amigos de la Universidad de Navarra 
3See 2

8:12AM Y14.00002 Kinetics of formation and disintegration of ionic and non-ionic spherical micelles1 , GUNJAN MOHAN, PPG Industries, DMITRY KOPELEVICH, University of Florida — Dynamics of self-assembly and structural transitions in amphiphilic systems play an important role in various industrial and biological processes. Main challenge in computational modeling of these dynamics is a complex interplay between various length- and time-scales. In this talk, we discuss development of a multi-scale model for formation and disintegration of non-ionic and ionic spherical micelles. This study is performed under the assumption that the dominant mechanism of micelle formation (disintegration) is a stepwise addition (removal) of individual surfactant monomers to (from) a surfactant aggregate. A series of molecular dynamics simulations is used to develop reduced stochastic models for these elementary processes. It is demonstrated that these processes involve complex interactions of the translational degree of freedom (i.e., distance between centers of mass of the aggregate and the monomer) with degrees of freedom corresponding to the monomer orientation and the micellar shape and microstructure.

1This research is supported by NSF
from evaporation at a pinned contact line. Our results suggest that dip-coating with control of dipping speed and evaporation rate produces unique assembled substrate. Surfactant concentration constantly increases in this confined environment due to solvent evaporation. Monodisperse crystalline islands nucleate monolayer of surfactant along the emerging solid-vapor interface. Above a critical contact line speed, an evaporating thin film is entrained on the emerging such as spin coating and dip coating. In this study, we demonstrate that altering the flow field near such a contact line fundamentally changes the deposited University, GUENNADI EVMENENKO, Northwestern University — Moving contact lines are often used to deposit soluble organic molecules in applications, BENJAMIN BEPPLER, KALYANI VARANASI, STEPHEN GAROFF, KRISTINA WOODS, Carnegie-Mellon University; GUENNADI EVMENENKO, Northwestern University — Moving contact lines are often used to deposit soluble organic molecules in applications, such as spin coating and dip coating. In this study, we demonstrate that altering the flow field near such a contact line fundamentally changes the deposited surfactant structure. At slow contact line speeds, the substrate emerges dry. The rolling fluid motion near the contact line deposits a densely packed, tilted monolayer of surfactant along the emerging solid-vapor interface. Above a critical contact line speed, an evaporating thin film is entrained on the emerging substrate. Surfactant concentration constantly increases in this confined environment due to solvent evaporation. Monodisperse crystalline islands nucleate and grow on the surface with sizes and shapes controlled by varying the deposition conditions. These results contrast with disordered deposits that result from evaporation at a pinned contact line. Our results suggest that dip-coating with control of dipping speed and evaporation rate produces unique assembled structures and may provide better control of deposition through moving contact lines.

Rapid Convective Deposition For Fabrication of Microlens Arrays . JAMES GILCHRIST, PISIST KUMNORKAEW, Department of Chemical Engineering, Lehigh University, NELSON TANUSI, YIK-KHOON EE, Department of Electrical and Computer Engineering, Lehigh University — Micron-sized microspheres were deposited into thin films via rapid convective deposition, similar to the ‘coffee ring’ effect, using a shear flow method that was developed by Prem and Velev, Langmuir, 2003. By varying deposition rate, evaporation rate, and solvent content, we show that high quality particles can be deposited in 2D close-packed arrays of microspheres existed. Obtained models do not consider the effect of blade angle and blade surface energy on the deposition rate. Using a confocal laser scanning microscope, dynamic self-assembly of colloidal particles under capillary force during solvent evaporation was revealed. The resulting microstructure controlled by varying the macroscale parameters and interaction between substrate and colloidal particles played an important role in formation of ordered crystalline arrays. These interactions were explored through a model comparing the residence time of a particle in the thin film and the characteristic time of capillary-driven crystallization to describe the morphology and microstructure of deposited particles. Fabricated microlens arrays assembled on LEDs using this process were demonstrated to enhance performance by 300%.

Permanently Flow-Induced Phase Transitions in Wormlike Surfactant Micelle Solutions , MUKUND VAŞĻDEVAN, Cytec Industries Inc. Stamford, CT, ERIC BUSE, Washington University, Saint Louis, MO, AMY SHEN, University of Washington, Seattle, WA, BAMIL KKHUMAMI, University of Tennessee, Knoxville, TN, RADHAKRISHNA SURESHKUMAR, Washington University, Saint Louis, MO — It is well known that certain wormlike micelle solutions form flow-induced structures under shear flow. This structure transition is typically accompanied by an enhancement in the shear viscosity and the emergence of a new gel phase. However, such transitions are generally believed to be reversible, i.e., upon flow stoppage, the structure relaxes to equilibrium. In this work, we show that by subjecting translucent wormlike micelle solutions to high flow deformation over a rapid time scale, permanent flow-induced structures can be formed. We will discuss the phenomenology and plausible physical mechanisms underlying this discovery.

Using fluid flow to control the structure of soluble surfactants deposited through receding contact lines . BENJAMIN BEPPLER, KALYANI VARANASI, STEPHEN GAROFF, KRISTINA WOODS, Carnegie-Mellon University, GUENNADI EVMENENKO, Northwestern University — Moving contact lines are often used to deposit soluble organic molecules in applications, such as spin coating and dip coating. In this study, we demonstrate that altering the flow field near such a contact line fundamentally changes the deposited surfactant structure. At slow contact line speeds, the substrate emerges dry. The rolling fluid motion near the contact line deposits a densely packed, tilted monolayer of surfactant along the emerging solid-vapor interface. Above a critical contact line speed, an evaporating thin film is entrained on the emerging substrate. Surfactant concentration constantly increases in this confined environment due to solvent evaporation. Monodisperse crystalline islands nucleate and grow on the surface with sizes and shapes controlled by varying the deposition conditions. These results contrast with disordered deposits that result from evaporation at a pinned contact line. Our results suggest that dip-coating with control of dipping speed and evaporation rate produces unique assembled structures and may provide better control of deposition through moving contact lines.

8:36 AM Y14.00004 Permanent Flow-Induced Phase Transitions in Wormlike Surfactant Micelle Solutions . MUKUND VAŞĻDEVAN, Cytec Industries Inc. Stamford, CT, ERIC BUSE, Washington University, Saint Louis, MO, AMY SHEN, University of Washington, Seattle, WA, BAMIL KKHUMAMI, University of Tennessee, Knoxville, TN, RADHAKRISHNA SURESHKUMAR, Washington University, Saint Louis, MO — It is well known that certain wormlike micelle solutions form flow-induced structures under shear flow. This structure transition is typically accompanied by an enhancement in the shear viscosity and the emergence of a new gel phase. However, such transitions are generally believed to be reversible, i.e., upon flow stoppage, the structure relaxes to equilibrium. In this work, we show that by subjecting translucent wormlike micelle solutions to high flow deformation over a rapid time scale, permanent flow-induced structures can be formed. We will discuss the phenomenology and plausible physical mechanisms underlying this discovery.

9:00 AM Y14.00006 Understanding the structure of porous materials created by freeze casting . STEPHEN BARR, ERIK LUIJTEN, University of Illinois at Urbana-Champaign — When a suspension of colloidal particles in water freezes, dendrites of ice with high aspect ratios are formed which can either engulf or reject the particles based on their size and the velocity of the advancing ice front. As the particles are pushed between the dendrites, concentrated regions of colloidal particles are formed. Recent experiments have shown that these regions can be exploited to create strong, lightweight, porous materials. We investigate this process using molecular dynamics simulations, focusing on the effect of the ice front velocity on the structure of the resulting material. We develop a simulation model which accounts for particle engulfment or rejection by the dendrites. We study both columnar and lamellar geometries. Our main finding is that variation of the front velocity not only affects the particle concentration in the interdendritic regions, but also the degree of order in the result structure.

End-Functionalized Triblock Copolymers as a Guide for Nanoparticle Ordering . RASTKO SKNEPNJEK, JOSHUA ANDERSON, MONICA LAMM, JOE R SCHMALIAN, ALEX TRAVESSET, Iowa State University and Ames Laboratory — Using molecular dynamics simulations we show that triblock copolymers, designed to have specific affinity for nanoparticles at the chain ends, can successfully mediate assembly of nanoparticle/copolymer composites. In this talk, we will present a detailed investigation of the phase diagram of these nanocomposites as a function of both nanoparticle size and concentration. We find a rich phase diagram with two striking features. The first is the existence of an unconventional square columnar phase of two interpenetrating line-lattices of micellar cylinders and aligned nanoparticles, and the second is a drastically enhanced stability of the gyroid phase. We interpret the origin of the square columnar phase by making an analogy to the packing of binary mixtures of disks. Based on the analysis of stretching of copolymers we argue that nanoparticles help stabilize gyroid order and drastically widen the region of its stability. Our study suggests that combining nanoparticles with functionalized block copolymers can provide a simple and efficient tool for assembling novel materials with nanometer scale resolution.

Unexpectedly wide distributions in the stochastic synthesis of functionalized nanoparticles . JACK WADDELL, DOUGLAS MULLEN, BRADFORD ORR, MARK BANASZK HOLL, LEONARD SANDER, University of Michigan — Functionalized nanoparticles are promising devices with a variety of applications, such as the targeted delivery of chemotherapy drugs to cancer cells. Their properties depend on the specifics of the distribution of functional groups on the nanoparticle. Stochastic ligand conjugation is an efficient strategy for synthesizing large quantities of functionalized nanoparticles. We developed a kinetic model for the study of ligand distribution on a generation 5 poly(aminodiamine) dendrimer, as measured by HPLC and SPR. We found a cooperative effect in single species ligation, leading to a broader-than-Poisson distribution of ligands on nanoparticles, and suggesting a high spatial correlation of functional groups.

9:24 AM Y14.00008 Self-assembly of silica nanoparticles in a surfactant mesophase . K. SHARMA, Ph.D. student; K. GURUSWAMY, Scientis; O. MONDA-MONVA, Professor, I. LY — We examine the organization of silica particles in a hexagonal mesophase of a non-ionic surfactant, C12E8 in water. The mesophase has a characteristic length scale (cylinder center-to-center distance, a ~ 5.7 nm). We vary the size of the silica particles from ∼ 2 nm (< a) to ∼500 nm (>> a), to examine the effect of particle size, and use a combination of SAXS, freeze fracture TEM and optical microscopy to characterize our materials. We show that particles < a behave like a solvent and template the mesophase. Particles with a size ~ a are partitioned into a dispersed phase and into strand-like aggregates. Particles > a phase separate from the mesophase and form strand-like aggregates that organize into a network. The formation of this network is reversible and heating into the high temperature isotropic phase leads to dispersion of the particles. Unusually an increase in hexagonal-isotropic transition temperature is seen for the mesophase-particle composites. We show that the network forms by expulsion of the particles from growing hexagonal phase domains as these domains grow, the particles are concentrated in the isotropic regions until they jam to form the network. We show that we are able to tune the mesh size of the particulate networks by changing the cooling rate.

8:24 AM Y14.00003 Using fluid flow to control the structure of soluble surfactants deposited through receding contact lines . BENJAMIN BEPPLER, KALYANI VARANASI, STEPHEN GAROFF, KRISTINA WOODS, Carnegie-Mellon University, GUENNADI EVMENENKO, Northwestern University — Moving contact lines are often used to deposit soluble organic molecules in applications, such as spin coating and dip coating. In this study, we demonstrate that altering the flow field near such a contact line fundamentally changes the deposited surfactant structure. At slow contact line speeds, the substrate emerges dry. The rolling fluid motion near the contact line deposits a densely packed, tilted monolayer of surfactant along the emerging solid-vapor interface. Above a critical contact line speed, an evaporating thin film is entrained on the emerging substrate. Surfactant concentration constantly increases in this confined environment due to solvent evaporation. Monodisperse crystalline islands nucleate and grow on the surface with sizes and shapes controlled by varying the deposition conditions. These results contrast with disordered deposits that result from evaporation at a pinned contact line. Our results suggest that dip-coating with control of dipping speed and evaporation rate produces unique assembled structures and may provide better control of deposition through moving contact lines.
8:00AM Y15.00001 Magnetic-field induced isotropic to nematic liquid crystal phase transition, J.T. GLEESON, T.B. OSTAPENKO, Kent State University, D. B. WIANT, Wake Forest University, S.N. SPRUNT, A. JAKLI, Kent State University — We report on measurements of magnetic field induced nematic order in the bent-core liquid crystal 4-chlororesorcinol bis-[4- (4-n-dodecylxiloxyzyl) benzolate]. Using the 31 Tesla solenoid at the National High Magnetic Field Laboratory, we have observed, at temperatures less than one degree above the clearing point, a first-order transition to the nematic phase. The critical magnetic field at which this occurs increases with temperature. We discuss these results within the context of both Maier-Saupe and Landau-deGennes mean field models for the nematic-isotropic transition. The implications of possible tetrahedral order are also discussed. To our knowledge, this is the first observation of such a magnetic field-induced transition in a thermotropic liquid crystal; the reasons for which this behavior is now attainable are discussed. This work was supported by the NSF (DMR-0606160) and Kent State University. Work performed at NHMFL supported by NSF cooperative agreement DMR-0084173, the State of Florida and the DOE.

8:12AM Y15.00002 High Magnetic Field-Induced Birefringence in Lyotropic Chromonic Liquid Crystals, T. OSTAPENKO, Kent State University, Y. NASTISHIN, Inst. for Phys. Opt., Lviv, Ukr., J.T. GLEESON, S.N. SPRUNT, O.D. LAVRENTOVICH, Kent State University, P.J. COLLINGS, Swarthmore College — We studied the effect of magnetic-field induced birefringence of a 14% solution of Sodium cromoglycate (DSCG) in water at temperatures above the nematic-isotropic coexistence region. According to Landau-deGennes mean field theory, we expect to find a linear relationship between the inverse of the induced birefringence, ∆n, and the quantity (T-T*)2, where T* is the stability limit of the isotropic phase. Using the 31 T resistive magnet at the National High Magnetic Field Laboratory, we observed that, as we increase the temperature above the coexistence region, we deviate from this linear dependence. Our data shows that ∆n goes to zero, whereas Landau-deGennes predicts that ∆n should decrease asymptotically. This may be due to the lack of isodesmic aggregate formation at a finite temperature above the coexistence region. Supported by NSF (DMR-0710544 and DMR-0606160). Work performed at NHMFL, supported by NSF cooperative agreements DMR-0084173, the State of Florida and the DOE.

8:24AM Y15.00003 ABSTRACT WITHDRAWN —

8:36AM Y15.00004 Chromonic liquid crystalline properties of dyes, XUXIA YAO, JUNG PARK, School of Polymer, Textile, and Fiber Engineering, Georgia Institute of Technology, MOHAN SRINIVASARAO, School of Polymer, Textile, and Fiber Engineering, School of Chemistry and Biochemistry, Georgia Institute of Technology — As a new class of lyotropic liquid crystals, chromonic liquid crystals (CLCs) can self-assemble into an ordered complex fluid, potentially useful for organic solar cells. Different from common amphiphilic lyotropic mesophases, CLCs have no optimum aggregation size, which implies the order parameter increases with concentration. We used capillary flow and magnetic field to induce alignment in chromonic dyes and studied the aggregation behavior by Vis-spectroscopy, the phase behavior by POM and DSC, and the order distribution by Raman Scattering. We also investigated how the molecular structures influence the structures of mesogens and the morphology in the dried film which will further influence the charge mobility in the solar cells.

8:48AM Y15.00005 Liquid Crystalline Phase Transition of Colloidal Platelets with Identical Thickness, DAZHI SUN, ZHENDONG CHENG, HUNG-JUE SUE, Texas A&M University, PROF. SUE’S TEAM, PROF. CHENG’S COLLABORATION — The disorder — order transition in discotic colloids has been an active research area since the observation of the nematic phase in clay suspensions by I. Langmuir in 1938. In the past decade, synthetic platelets have been used extensively to investigate the discotic liquid crystal phase transitions. Here, we report the phase behavior of a new model platelet system — alpha-zirconium phosphate (ZrP). After exfoliation, the monolayer ZrP platelets possess uniform thickness, but have a high polydispersity in diameter. We observed an isotropic — nematic transition in our system upon increasing the platelet volume fraction, followed by the formation of the discotic smectic phase, an elusive phase that has been rarely seen in discotic liquid crystals. The discotic smectic phase (domain) is characterized by X-ray diffraction, high-resolution transmission electron microscopy, and optical microscopy. The equation of state (EOS) of our system is also discussed.

1 Special thanks are given to The Dow Chemical Company for their partial financial support. Acknowledgment is also made to the donors of the American Chemical Society ACS Petroleum Research Fund (RPF9-43053-G7).

9:00AM Y15.00006 Study of the Isotropic-Nematic and the Nematic-Smectic-A Phase Transitions in Carbon Nanotubes and Liquid Crystal Composites, KRISHNA SIGDEL, GERMANO IANNACCIONE, Worcester Polytechnic Institute — A high-resolution ac calorimetric study of the isotropic to nematic (I-N) and the nematic to smectic-A (N-SmA) phases transitions of carbon nanotubes (CNTs) and liquid crystal octyl-cyanobiphenyl (8CB) composites (8CB+CNTs) as a function of CNTs concentration is reported. Scans were performed on heating and cooling for all samples (0.5-6 wt% of CNTs) over a wide temperature range well above and below the two transitions in pure 8CB. Both the I-N and the N-SmA transitions evolve in character and have their transition temperatures shift lower as the wt% of CNTs increases. For intermediate wt% values, new transitions features are observed, which suggest new phase ordering of the CNTs within the liquid crystal host.

9:12AM Y15.00007 Recovery and stabilization of a reversed phase sequence in a ternary liquid crystal mixture, RONALD PINDAK, Brookhaven National Lab, SHUN WANG, LIDONG PAN, Univ. of Minnesota, B.K. MCCOY, Azusa Pacific Univ., SUNTAO WANG, Brookhaven National Lab, H.T. NGUYEN, Univ. Bordeaux, CHENG-CHER HUANG, Univ. of Minnesota — The nCHFBB1M7 (n = 10) compound, 100HF, shows a reversed SmC*F12 – SmC* phase sequence, unique among all known antifluoroelastic liquid crystals. This reversed phase sequence is stabilized upon doping with 9OTBBB1M7(C9) or 11OTBBB1M7(C11). One 100HF/110HF mixture without the SmC*F12 phase was selected for further studies. Adding C9 into this mixture revives the reversed phase sequence. Unexpectedly, even though 110HF destabilizes the SmC*F12 phase in binary mixtures with 100HF, it significantly increases the SmC*F12 temperature range in 100HF/110HF/C9 ternary mixtures. The extended temperature range is important for device applications.

9:24AM Y15.00008 Room-Temperature Liquid Crystal Blue Phases, STEFANIE TAUSHANOFF, Kent State University, KHOA VAN LE, Tokyo Institute of Technology, ROBERT TWIEG, ANITAL JAKLI, Kent State University — The “blue phases” of a highly chiral liquid crystal are defect-studied structures of double-twist cylinders that are laced together. The three phases, BPII*, BPIII*, and BPIII** differ only in the packing of the double-twist cylinders. Until recently, blue phases were of limited practical use because they appeared for only a very narrow temperature range. Mixtures that show BPII* and BPIII* phases for wide temperature ranges at or around room temperature are now available [1]. Relatively wide temperature BPIII (the blue fog) phase so far was available only at very high temperatures [2]. Here we present mixtures with room-temperature wide range BPIII phase and compare the ability of chiral dopants to form the different blue phases in a base nematic mixture. PDLC films cast with blue-phase material are also examined.

9:36AM Y15.00009 Hybrid shells of nematic liquid crystal, ALBERTO FERNANDEZ-NIEVES, TERESA LOPEZ-LEON, Georgia Tech — We investigate the consequences of changing the boundary conditions for the nematic director at the outer surface of a spherical shell from planar to homeotropic. We find there are different routes to the final equilibrium configuration, depending on the initial shell structure. For bipolar shells, which are shells having two pairs of $s=+1$ boojums on either surface, a disclination ring forms, shrinks and disappears in a process that is highly reminiscent of that seen in bipolar drops. By contrast, shells with four $s=+1/2$ defects develop open disclination lines in the inner surface; these lines form between the original $s=+1/2$ defects and force their approach and coalescence. These results highlight the fascinating range of behaviors that are driven by the interplay between topological constraints and the nematic order of liquid crystals.

9:48AM Y15.00010 Optical waveguiding in bent core liquid crystal filaments, ANTAL JAKLI, JAKE FONTANA, CHRIS BAILEY, Kent State University, Kent, OH, USA, WOLFGANG WEISSFLOG, Martin Luther University, Halle, Germany, ISTVAN JANOSSY, Research Inst. for Solid State Physics and Optics, Budapest, Hungary, PETER PALFFY-MUHORAY, Kent State University, Kent, OH USA — We demonstrate optical waveguiding in recently discovered free-standing bent core liquid crystal filaments. The bent core liquid crystal molecules self-assemble into a novel cylindrical geometry that is “solid-like” in the radial direction of the filament and liquid in the axial direction of the filament. Waveguiding properties of filaments of millimeter lengths were characterized. The transmitted power density through the filament was independent of temperature from 180°C to near room temperature. Initial defect of newly pulled filaments were found to self-annex, thus leaving perfectly defect free fibers, where light scattering was found to be insignificant. The absorbance was found to be strongly wavelength dependent in the visible regime and very small in the infrared range. A self-assembled optical waveguide with self-annelling fluid properties may have promising applications in optical communications.

This work was supported by NSF IRES OISE-0727185.

10:00AM Y15.00011 Dielectric properties of bent-core nematic materials, PETER SALAMON, NANDOR EBER, SAMUEL SPRUNT, JAMES GLEESON, ANTAL JAKLI — We report of dielectric spectroscopy measurements on bent-core nematic liquid crystals. The components of the relative dielectric permittivity and the dielectric loss have been measured as functions of frequency and temperature in the case of various bent-core mesogens in their nematic and isotropic phases. The results show that these liquid crystals have extraordinary dielectric behaviors if we compare them to the traditional calamitic materials, such as they show low frequency (<10 KHz) relaxations. Distortion elastic constants measurements reveal that $K_1 / K_3 \sim 1$ in contrast to typical calamitics. The reasons for these anomalous behaviors will be discussed.

This work was supported by NSF DMR 0006160, and OTKA-K-61075.

10:12AM Y15.00012 Second Harmonic Generation in a Bent-core Nematic Liquid Crystal, SEUNG HO HONG, ANTAL JAKLI, JAMES GLEESON, SAMUEL SPRUNT, BRETTT ELLMAN, Kent State University — We studied second harmonic generation (SHG) as a function of optical polarization in a magnetically-aligned bent-core nematic liquid crystal (BCN). At the isotropic to nematic transition we detect the onset of a weak SH signal, which stays approximately constant through the nematic phase. Our results for polarization selectivity and for cells of different thickness indicate that the signal from the BCN cannot be explained by quadrupoles, defects in director orientation, fluctuations or cell-surface polarization. We discuss models for a noncentrosymmetric component of the BCN structure that can explain our data.

1This work was supported by NSF DMR0606160.

10:24AM Y15.00013 Viscoelastic parameters and flexoelectric effect in a bent-core nematic liquid crystal studied by dynamic light scattering, MADHABI MAJUMDAR, K. NEUPANE, JAMES T. GLEESON, ANTAL JAKLI, SAMUEL SPRUNT, Kent State University — Recent measurements of the flexure-induced electric polarization in certain bent-core nematics (BCNs) have demonstrated a giant flexoelectric effect [1]. We present a study of nematic elasticities and viscosities in one of these compounds, together with an attempt to characterize the flexoelectricity by its effect on director fluctuations. Our results combined with a reanalysis of earlier data indicate that the flexoelectricity is a phenomenon distinct from the ordinary director modes; additionally we observe unusual, very slow fluctuations in polarized scattering which suggest the BCN has a heterogeneous, “glassy” character. Dilution in a miscible calamitic indicates a dramatic development of the slow dynamics between 30 wt % and 60 wt % BCN. We suggest a model to account for both our present results and the giant flexoelectricity discovered in [1]. Reference: [1] J. Harden et al., Phys. Rev. Lett., 97, 157802 (2006). Acknowledgement: NSF DMR-0606160.

10:36AM Y15.00014 Large Flow-Birefringence of Nematogenic Bent-Core Liquid Crystals, CHRISTOPHER BAILEY, Kent State University, KATALIN FODOR-CSORBA, Research Institute for solid state physics and optics, Budapest, Hungary, RAFAEL VERDUZCO, Oak Ridge National Laboratory, JAMES GLEESON, SAMUEL SPRUNT, ANTAL JAKLI, Kent State University — We have found that bent-core liquid crystalline materials show exceptionally large flow birefringence in their isotropic liquid phase. The flow birefringence is over two orders of magnitude larger than low molecular weight and side-chain polymeric calamitic liquid crystals. This large flow birefringence is attributed to the nanostructure that bent-core liquid crystalline materials show exceptionally large flow birefringence in their isotropic liquid phase. The flow birefringence is over two orders of magnitude larger than low molecular weight and side-chain polymeric calamitic liquid crystals. This large flow birefringence is attributed to the nanostructure.

10:48AM Y15.00015 Activated Kinetics of Nematic and Smectic Phase Transitions in an Aligned Matrix of Nano-colloidal Liquid Crystalline Gel, DIPTI SHARMA, UML — This study investigates an interesting thermal behavior of an aligned aerosil nano-colloidal system in the aligned matrix of octyl-cyanobiphenyl liquid crystal. This system was prepared by solvent dispersion method (SDM) where different densities of aerosil nanoparticles were added into octyl-cyanobiphenyl liquid crystal. Then samples were cycled into magnetic field during SmA-I transition to get an aligned matrix of nanocolloids. Heating scans were performed at various heating rates from 20 to 1 K min$^{-1}$ using DSC. Aligned samples follow Arrhenius behavior and showed a decrease in transitions temperature for SmA–N and N–I transitions when compared with the unaligned samples. The activation energy of the aligned system increases and its respective enthalpy decreases for the lowest density of aerosils 0.05 g cm$^{-3}$, then for the further increase of aerosil density, the activation energy decreases and its respective enthalpy increases. The second order transition SmA–N shows a higher activated kinetics than the weak first order N–I transition. This can be explained in terms of molecular interaction in between aerosil nanoparticles and aligned liquid crystal molecules, and developed strain in the matrix of the aligned system.

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Corrections affect the thermodynamic stability of bicontinuous mesophase structures, such as gyroid. The interparticle potential. Finally, we discuss the finite-temperature corrections to strong segregation theory in terms of Sommerfeld-like expansion and how these produce a phase diagram including Lamella, Hexagonal-columnar, and BCC phases, and their inverse phases in the parameter space of chemical potential and possible aggregate structures associated with the spatially modulated field, together with a half-filling condition at the interface of morphology, allows us to forming a variety of mesophases. We combine a mean field theory developed from a lattice model with a level surface analysis of the periodic structures of SANTANGELO, University of Massachusetts, Amherst — Soft spheres interacting via a hard core and purely repulsive shoulder self-assemble into clusters even at very low volume fractions of the fluorinated segments. The micelles exhibit unique temperature stability in comparison with aggregates formed by siloxane segment. The high degree of segregation results in association into star-like micelles with the fluorinated siloxane in the core and a swollen corona (PTFPMS-PS) in solutions of d the current work introduces a small angle neutron scattering study of a highly segregated diblock-copolymer, a trifluoro propylmethyl siloxane - polystyrene experimental and theoretical studies have investigated solutions of diblocks with a relatively low incompatibility, requiring relatively large blocks to associate. association of diblock co-polymers in selective solvents. The shape of the micelles is affected by the size of the blocks and their interaction with the solvent. Most experimental and theoretical studies have investigated solutions of diblocks with a relatively low incompatibility, requiring relatively large blocks to associate. The current work introduces a small angle neutron scattering study of a highly segregated diblock-copolymer, a trifluoro propylmethyl siloxane - polystyrene (PTFPMS-PS) in solutions of d-toluene, a good solvent for the polystyrene. Studies were carried out over volume fractions of 0.1 to 0.5 of the fluorinated siloxane segment. The high degree of segregation results in association into star-like micelles with the fluorinated siloxane in the core and a swollen corona even at very low volume fractions of the fluorinated segments. The micelles exhibit unique temperature stability in comparison with aggregates formed by diblock-copolymers in a lower segregation regime. The detailed structure of these aggregates as a function of volume fraction and temperature will be discussed. The rise to self-assembled hierarchical structures such as tapes, ribbons and fibrils, which at sufficiently high concentrations form nematic liquid crystalline solutions and gels. Applications of these novel materials are found in nanotechnology, medicine and personal care products. Such aggregates not only appear in the context of desirable biomaterials but also in pathological self-assembly of mis-folded proteins, forming aggregates such as “amyloids”. Recently a theoretical model was developed to understand the properties of these self-assembling structures [1]. The question which arises is what happens if we mix different peptide species varying e.g. in length or interaction energy. Do they mix in self-assembled structures or form separate ones? This is of crucial importance as most of industrially produced materials are not monodisperse. To model the simplest polydisperse system, we apply two-component self-assembled Ising model, in which three energy scales are involved. We show that depending upon the relative values of these energy scales and concentrations of the two components, different morphologies of tapes consisting of both components are formed exhibiting paramagnetic, ferromagnetic or antiferromagnetic order. [1] A. Aggeli, et al; PNAS 2001, 98, 11857

We would like to acknowledge DPI for funding this project.

Self-assembly induced protein crystallization, HONGJUN LIU, SANAT KUMAR, Columbia University, JACK DOUGLAS, NIST — The strongly anisotropic nature of inter-protein interactions naturally leads them to self-assemble into structures mirroring the symmetry of the inter-protein potential. Self-assembly is a thermodynamically distinct phenomenon from phase separation, and we consider whether it can play a direct role in nucleating protein crystallization. Previous simulations and measurements have established that protein clusters formed below the critical point for liquid-liquid phase separation (Tc) can facilitate crystal nucleation. However, recent experiments have indicated the existence of clustering-induced protein nucleation even for T > Tc, where phase separation does not exist. Here we simulate a minimal model of patchy particles and indeed find that transient clusters formed through self-assembly (even above Tc) can nucleate crystal growth. Importantly, the self-assembled clusters help to select the symmetry of the resulting crystal growth. In contrast, protein crystallization for T < Tc does not have this directing influence, and polycrystalline growth forms, such as spherulites, are then prevalent. Our simulations suggest that self-assembly directed crystallization might be common in protein solutions and that this process is relevant for understanding protein crystallization polymorphism.

Mechanisms for semi-flexible filament self-assembly: an experimental and simulation study, LAM NGUYEN, Center for Materials Research and Technology (MARTECH), Department of Physics, Florida State University, WEI YANG, STEVE ACQUAH, HAROLD KROTO, Department of Chemistry & Biochemistry, Florida State University, LINDA HIRST, School of Natural Sciences, University of California, Merced — The self-assembly of semi-flexible filaments, such as F-actin, in the presence of cross-linkers has been studied experimentally and via molecular dynamics simulation. Several imaging techniques including fluorescence and electron microscopy have been used to elucidate the structural properties of formed bundles and networks of filaments. We are able to observe the dynamical process of the self-assembly and study the driving forces behind filament aggregation. The roles of different parameters such as cross-linker density and filament length have been investigated, determining the assembled system properties. We find both of these parameters to play a key role in the final structure formation. Understanding the mechanism for the self-assembly of these semi-flexible filaments will be very useful in the application of developing a new class of biological materials.

Computer simulations of the self-assembly of chiral superstructures from rigid achiral constituents, CHRISTOPHER HIXSON, FAN YANG, DAVID EARL, Department of Chemistry, University of Pittsburgh — We present the results of computer simulations of an achiral rigid bent-core model system at a range of temperatures and densities. We observe nematic and smectic phases, but more interestingly observe chiral micelles and columns at lower densities. The origin of these chiral features are explored using minimization techniques and parallel tempering searches. We show that chiral structures are minima of the potential energy surface. Additionally, we show that the addition of chiral dopant induces the system to order into a single twist direction.

Computer simulations of the self-assembly of chiral superstructures from rigid achiral constituents, CHRISTOPHER HIXSON, FANGYONG YAN, DAVID EARL, Department of Chemistry, University of Pittsburgh — We present the results of computer simulations of an achiral rigid bent-core model system at a range of temperatures and densities. We observe nematic and smectic phases, but more interestingly observe chiral micelles and columns at lower densities. The origin of these chiral features are explored using minimization techniques and parallel tempering searches. We show that chiral structures are minima of the potential energy surface. Additionally, we show that the addition of chiral dopant induces the system to order into a single twist direction.

Reversible pH-Induced Structural Transition in a Polyelectrolyte-Surfactant System: from Semi-flexible Rod to String of Spheres, VIET LAM, LYNN WALKER, Carnegie Mellon University — We have characterized a polyelectrolyte-surfactant system that forms stable rod-like aggregates in aqueous solution. While this structure is stable to most changes in solution condition, we have observed a reversible change in behavior with pH. This is due to a pH-induced structural transition from the original semi-flexible rod at neutral pH to a more flexible object at acidic conditions. A simple model of polyelectrolyte chain crossing multiple surfactant spherical micelles, or a string of spheres, has been proposed as the structure of the aggregates at low pH. This represents a novel rod-like nanoscale system that goes through a reversible gelation with pH, with possible use in oil drilling (matrix acidification aid), liquid flow control, or transport of hydrophobic materials. Here, we will present a simple model of the structural change and experimental justification.

Self-Assembly of Highly Segregating Diblock Copolymer in Solution, DILRU RATNAWEERA, Clemson University, STEPHEN CLARSON, University of Cincinnati, DVORA PERAHIA, Clemson University — We have characterized a polyelectrolyte-surfactant system that forms stable rod-like aggregates in aqueous solution. While this structure is stable to most changes in solution condition, we have observed a reversible change in behavior with pH. This is due to a pH-induced structural transition from the original semi-flexible rod at neutral pH to a more flexible object at acidic conditions. A simple model of polyelectrolyte chain crossing multiple surfactant spherical micelles, or a string of spheres, has been proposed as the structure of the aggregates at low pH. This represents a novel rod-like nanoscale system that goes through a reversible gelation with pH, with possible use in oil drilling (matrix acidification aid), liquid flow control, or transport of hydrophobic materials. Here, we will present a simple model of the structural change and experimental justification.

Mesophases of soft-sphere aggregates, HOMIN SHIN, GREGORY GRASON, CHRISTIAN SANTANGELO, University of Massachusetts, Amherst — Soft spheres interacting via a hard core and purely repulsive shoulder self-assemble into clusters forming a variety of mesophases. We combine a mean field theory developed from a lattice model with a level surface analysis of the periodic structures of soft-sphere aggregates to study stable morphologies for a class of interaction potentials. The mean-field solution shows that the site occupation density and interparticle potential are self-consistently related to an “effective field” acting on each particle. In the strong segregation limit, the space group symmetry of possible aggregate structures associated with the spatially modulated field, together with a half-filling condition at the interface of morphology, allows us to produce a phase diagram including Lamella, Hexagonal-columnar, and BCC phases, and their inverse phases in the parameter space of chemical potential and interparticle potential. Finally, we discuss the finite-temperature corrections to strong segregation theory in terms of Sommerfeld-like expansion and how these corrections affect the thermodynamic stability of bicontinuous mesophase structures, such as gyroid.
12:39PM Z14.00008 Breaking it up: Simulations of micelle fission in explicit solvent, MIKKO KARTTUNEN, The University of Western Ontario, MARIA SAMMALKORPI, MIKKO HAATAJA, Princeton University — We study self-assembly in micellar systems consisting of sodium dodecyl sulfate (SDS) using detailed 200-400 ns atomic scale molecular dynamics simulations. The simulations were done with explicit solvent, counterions and salt. We focus on the role of molecular level interactions driving self-assembly [1] and, in particular, show how micelle fission can be controlled using electrostatics. As our main result, we demonstrate the existence of a new fission pathway in charged micelles [2] and provide a physical explanation for it.


12:51PM Z14.00009 Neutron Scattering Analysis of the Dynamics and Structure of Semiflexible, Self-Assembled Peptide Chain Networks and WormLike Micelles, N. WAGNER, M. BRANCO, D. POCHAN, J. SCHNEIDER, University of Delaware — Self assembled peptide hydrogels are formed from synthetic β-hairpin peptides that undergo triggered self assembly to form a physically crosslinked network of entangled fibrils. Upon salt addition at pH 7.4, these peptides fold into a β-hairpin self-assemble to form a rigid hydrogel stabilized by non-covalent crosslinks. A single amino acid substitution is performed to change the charge on the peptide and greatly alter the rate of assembly. As a result, faster folding and self assembly kinetics are observed leading to more rigid gels. Transmission electron microscopy (TEM) and rheology demonstrate that the resultant, rigid networks of the semiflexible fibrils are composed of a bilayer of hairpins with a cross-sectional diameter of 3 nm, corresponding to the width of a folded peptide. Neutron spin echo (NSE) measurements show that the peptides can be modeled as semiflexible chains on lengthsscales shorter than the characteristic mesh size. The chain diffusivity is reduced by the peptide substitution and this can be attributed to alteration of the electrostatic interactions between peptides in the fibril. Small angle neutron scattering (SANS) measurements show a transition from a cylindrical rod-like geometry to a more branched, fractal-like network topology upon amino acid substitution. These measurements explain the large increase in gel modulus observed upon amino acid substitution. These results facilitate the rational design of self-assembling peptide materials for biomaterial applications. NSE results for semiflexible wormlike micelles will also be discussed.

1:03PM Z14.00010 Chiral Self-Assembly of Rodlike Viruses, EDWARD BARRY, ZVONIMIR DOGIC, ROBERT MEYER, Brandeis University, ROBERT PELCOVITS, Brown University, RUDOLF OLDENBOURG, Marine Biological Laboratory — The self-assembly of two dimensional achiral membranes which occurs in entropic mixtures of monodisperse colloidal rods and non-adsorbing polymers will be described. The colloidal nature of the rod/polymer model system enables us to simultaneously examine the behavior of self-assembled membranes at both the molecular and continuum lengthscales. Combining observations made at the very different lengthscales, we investigate how chirality frustrates assembly of achiral 2D membranes altogether, and instead drives the formation of very complex and highly regular chiral structures. Representative structures obtained through chiral self-assembly include: twisted ribbons, double helices, two dimensional analogs of a TGB phase, and regular arrays of pores embedded within a 2D membrane.