DY 5: Soft Matter I

Time: Monday 15:00–17:30 Location: MA 004

DY 5.1 Mon 15:00 MA 004

Onset of flow in a confined model colloidal glass — •Pinaki Chaudhuri[1,2] and Juergen Horbach[1] — [1]Institut für Theoretische Physik II, Heinrich Heine-Universität Düsseldorf, Universitätsstr. 1, 40225 Düsseldorf, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany

Understanding the mechanisms that build up flow in soft glassy systems remains an outstanding problem. In recent times, because of various practical applications, flow of such systems under confinement has also drawn considerable attention. Using numerical simulations, we study the onset of flow, under confinement, in a model colloidal glass under an externally applied stress. Typically, amorphous systems yield when the stress exceeds a threshold value (the yield stress) - we show that the time-scales for the onset of steady state flow rapidly increase as the applied stress is lowered towards the threshold. Moreover we observe that, in confinement, these time-scales depend on the nature of the imposed stress - e.g, they are longer for a Poiseuille flow, compared to a Couette flow. We further elucidate the microscopic process that are responsible for these increasing time-scales as well as the differences with the various applied stress fields.

DY 5.2 Mon 15:15 MA 004

Capillary wave analysis of crystal-liquid interface in colloidal model systems — •Aleksandar Mijailovic, Roberto E. Rozas, Jürgen Horbach, and Hartmut Löwen — Institut für Theoretische Physik 2, Heinrich-Heine Universität Düsseldorf, Germany

The properties of the crystal-liquid interface of inhomogeneous colloidal systems is determined from molecular dynamic (MD) simulations. Interactions between particles are modeled by the Yukawa pair potential. As a test of consistency of the capillary waves theory (CWT) the interfacial stiffness is calculated for the (100) crystal orientation using two independent methods: (1) from the spectrum of capillary waves at the interface and (2) from the interfacial broadening-effect predicted by the theory [1, 2]. A complete mapping of the interfacial energy as a function of the crystal orientation from the spectrum of height-height correlation of different crystal orientations is obtained. The results obtained in appropriate units are comparable to the hard spheres case. In addition, the kinetic growth coefficients are estimated in growth simulations of different undercoolings.

DY 5.3 Mon 15:30 MA 004

Orientational dynamics of nematic liquid crystals under shear flow: Stability and growth of dynamical modes in inhomogeneous systems. — •David A. Strehober and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We study the nonequilibrium dynamics of rodlike nematic polymers under shear flow. We employ a mesoscopic description, and use the alignment tensor as an order parameter. Five coupled partial differential equations describe the dynamics of the alignment tensor [1][2]. The rheological phase diagram with respect to the shear rate and reduced temperature are investigated for the homogeneous case. We employ numerical continuation methods [3], to obtain the boundaries between different dynamic states. We also check the validity of the results for the 1D inhomogeneous case and discuss differences to the homogeneous case. We conclude the talk with results of the investigation of domain growth of dynamic states.

[1] S. Hess, Z.Naturforsch. A **31a**, 1034 (1976)
[2] S. Grandner, S. Heidenreich, S. Hess and S. H. L. Klapp, Eur.Phys.J. E **24**, 353 (2007)
[3] A. Dhooge, W. Govaerts, and Yu. A. Kuznetsov., ACM Trans. Math. Softw. **29**, (2003)

DY 5.4 Mon 15:45 MA 004

Crosslinker-induced formation of filament networks: Dependence on the filament length. — •Thomas Gruhn[1] and Raghunath Chelakkot[2] — [1]Material- und Prozesssimulation, Universität Bayreuth, D-95440 Bayreuth. — [2]Physics Department, Brandeis University, Waltham, MA-02454, USA.

Self-assembling networks of rod-like filaments are of technological and scientific interest. Due to their complex morphology and their huge internal surface area, they are excellently suited for nano-circuits, high efficiency catalysts, and molecular sensors. In the cytoskeleton of living cells, such networks are formed by F-actin filaments, which are interconnected by crosslinkers like myosin or α-actinin. We have analyzed the percolation behavior of a self-assembling network of rigid filaments and reversibly binding crosslinkers with the help of Monte Carlo simulations. In the system, filaments are represented by long spherocylinders, while crosslinkers are mimicked by short spherocylinders with adhesive sites at both ends with which the crosslinkers can bind to the filaments. In our recent studies we have studied the influence of the filament length on the percolation threshold. For a given filament volume fraction and crosslinker filament ratio, the network formation and the percolation threshold is remarkably independent of the filament length, while changes of the packing fraction have a distinct impact on the percolation threshold. The system behavior is analyzed with an analytical approach, which reproduces the binding probability qualitatively and provides a deeper insight into the basic aspects of network formation.

DY 5.5 Mon 16:00 MA 004

Dilatational yielding of solid Langmuir monolayers — •Saeedeh Aliaskarisohi[1], Thomas.M Fischer[1], and Natalia Wilke[2] — [1]University of Bayreuth,Bayreuth, Germany — [2]Universidad Nacional de Cordoba,Cordoba, Argentina

In a previous work, Muruganathan and Fischer observed laser induced local collapse of a methyl stearate monolayer. These experiments opened the possibility of studying the collapse mechanism in a highly controlled manner, since the laser intensity can be easily varied and collapse happens in a definite place (the laser focus). In this paper we extended the work presented by Muruganathan et al., describing the local yielding as an alternative pathway toward monolayer collapse competing with the global collapse of the monolayer. We first corroborated that the laser-induced collapse is a thermocapillary effect and afterward determined the threshold laser power necessary for the local pathway to win over the global collapse. We show that the laser threshold is determined more by the gradients in temperature and pressure than by the global pressure and temperature. We propose that the flow of material into the focus of the laser is observed after the yield stress of the monolayer is overcome. The higher the yield stress, the higher the temperature gradient that is necessary for the monolayer to yield. The local pathway opens only when the derivative of surface pressure with temperature is negative such that stress gradients point toward the laser focus and a sink of material is generated. In such a case we are able to give estimates of the dilatational yield pressure of the solid monolayer.

DY 5.6 Mon 16:15 MA 004

Molecular dynamics and morphology in confined 4-heptan-4-isothiocyanatobiphenyl liquid crystals — •Malgorzata Jasiurkowska[1], Wilhelm Kossack[1], Roxana Enea[1], Ciprian Iacob[1], Wycliffe Kipnusu[1], Periklis Papadopoulos[2], Joshua Sangoro[1], Maria Massalska-Arodz[3], and Friedrich Kremer[1] — [1]Institute of Experimental Physics I, University of Leipzig, Linnestr. 5, 04103 Leipzig, Germany — [2]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [3]The Henryk Niewodniczanski Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland

Molecular dynamics and orientational order of 4-heptan-4-isothiocyanatobiphenyl (7BT) confined in non-intersecting pores of mean diameters from 4 nm to 10.5 nm are studied by a combination of Broadband Dielectric and Fourier-Transform Infrared Spectroscopy. In contrast to well-known bulk dielectric properties of nBTs, confinement leads to modification of the molecular dynamics. Infrared Transition Moment Orientational Analysis reveals different molecular arrangement in pores of diameters 10.5 nm compared to the molecules enclosed in 4 nm and 6 nm diameter pores

DY 5.7 Mon 16:30 MA 004

Bicontinuous and mixed gels in binary mixtures of patchy colloidal particles — •Daniel de las Heras[1,2], Jose María Tavares[2], and Margarida Telo da Gama[2] — [1]Theoretische Physik II, Physikalisches Institut, Universität Bayreuth, Universitättsstraße

30, D-95447 Bayreuth, Germany — [2]Centro de Física Teórica e Computacional da Universidade de Lisboa, Avenida Professor Gama Pinto 2, P-1649-003, Lisbon, Portugal

We investigate the thermodynamics and percolation regimes of model binary mixtures of patchy colloidal particles [1]. The particles of each species have three interaction sites of two types, one of which promotes bonding of particles of the same species while the other promotes bonding of different species. We find up to four percolated structures at low temperatures and densities: two gels where only one species percolates, a mixed gel where particles of both species percolate but neither species percolates separately, and a bicontinuous gel where particles of both species percolate separately forming two interconnected networks. The competition between the entropy and the energy of bonding drives the stability of the different percolating structures.

Appropriate mixtures exhibit one or more connectivity transitions between the mixed and bicontinuous gels, as the temperature and/or the composition changes.

[1] D. de las Heras, J.M. Tavares, and M.M. Telo da Gama. Accepted for publication in Soft Matter, 2011. (http://arxiv.org/abs/1111.3741)

DY 5.8 Mon 16:45 MA 004

Dynamic phase behaviour of soft colloids — •Sudipta Gupta, Stellbrink Joerg, and Richter Dieter — JCNS1/ICS1, Forschungszentrum Juelich, 52425 Germany

Soft colloids, e.g. polymer-coated silica particles, block copolymer micelles, star polymers etc., are hybrids between (linear) polymer chains and (hard sphere) colloids. Due to this hybrid nature, soft colloids macroscopically show interesting (phase) behaviour resulting from its unique microscopic structure. We introduce kinetically frozen diblock copolymer micelles as an "easy-to-establish" and "tuneable" model system for soft colloids. The micellar architecture was tuned from the star-like to the crew-cut regime by varying the block-ratio. The micellar structure was successfully determined using SANS. At the same time, we are studying the flow properties both at semi-dilute and at concentrated regime for this different block ratio, using rheology. By constructing a dynamic phase diagram we can conclude that the macroscopic flow properties do strongly depend on the microscopic structure determined by SANS. Thereby we investigate the basic principles of the so-called structure-property-relationship (SPR) that finally enables tailoring material properties for technical applications. The change in block ratio significantly affects the phase behaviour of this particular class of soft colloids. A more detailed investigation of this phase behaviour is still under progress.

Topical Talk DY 5.9 Mon 17:00 MA 004

Phason dynamics in light-induced colloidal quasicrystals — •Michael Schmiedeberg[1], Justus Kromer[2], and Holger Stark[2] — [1]Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Institut für Theoretische Physik, Technische Universität Berlin, Germany

Quasicrystals are non-periodic solids which nevertheless possess long-range positional and orientational order. We study a 2D charge-stabilized colloidal suspension in an external potential with quasicrystalline symmetry. In experiments the potential is realized by five, seven, or more interfering laser beams. A short overview on the properties of light-induced colloidal quasicrystals is presented.

A distinctive physical property of quasicrystals are phasons, which correspond to correlated rearrangements of atoms throughout the quasicrystal. Phasons, like phonons, are hydrodynamic modes since they do not cost free energy in the long-wave-length limit. We perform Brownian dynamics simulations to unravel single-particle dynamics when a constant phasonic drift is applied to the quasicrystalline potential. Single colloids exhibit characteristic trajectories along different directions that are given by their starting positions. Properties of conventional crystals can be deduced from a single unit cell which does not exist in quasicrystals. Nevertheless, we are able to define a characteristic area for phononic and phasonic displacement. We demonstrate that each particle trajectory can then be predicted by mapping it into this area. Our observations help to get a deeper insight into the properties of phasonic displacements in colloidal as well as in atomic quasicrystals.