DY 17: Soft matter

Time: Wednesday 10:00–12:00 Location: H47

DY 17.1 Wed 10:00 H47

Particle tracking in drying colloidal films — Jan S. Vesaratchanon and •Lucas Goehring — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Colloidal dispersions, such as paints, coatings, inks, drops of wine or coffee, usually dry into either a uniformly flat surface or a dispersed phase that is deposited mostly at the edges forming a ring. This ring formation can be similarly observed elsewhere in the so called "coffee-ring effect". However, the conditions which select for these two extreme cases, or an intermediate deposit, are not known. Furthermore, understanding the basic transport and flow properties during the drying process can be useful in many industrial applications. We use a particle tracking microscopy technique in order to investigate the motion of particles during drying. By adding fluorescent particles as tracers into drying colloids of relatively similar particle size, we are able to extract the trajectories of individual fluorescent particles along with their coordinates and time. Our experimental setup allows us to measure drift velocity of individual particles approaching a solidification front, along with drying front velocity (i.e., how fast colloids dry), particle density and self-diffusion parameters. Variation of particle size and drying rate during experiments allows us to understand the scaling of key parameters relevant to the drying of colloidal films.

DY 17.2 Wed 10:15 H47

Model System for the Random Organization and Jamming Transition — •Lars Milz[1,2] and Michael Schmiedeberg[2] — [1]Universität Regensburg, 93053 Regensburg, Germany — [2]Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40204 Düsseldorf, Germany

Random organization is a non-equilibrium phase transition between a steady state and an absorbing state. This transition was observed in a system with periodically sheared non-Brownian particles where at low densities or low shear amplitudes the particle organize such that collisions are avoided while at large densities or large shear amplitudes collisions still occur [1,2]. We consider a simplified model system without shear where in each step particles are displaced if they overlap. For displacements in random directions we observe the random organization transition and explain how the shear amplitude and density in [1,2] can be mapped onto the packing fraction, which is our only control parameter. Interestingly, for deterministic displacements we find crystallization in 2D and the jamming transition in 3D. Therefore, our model system provides a simple method to study the random organization transition and a link between this non-equilibrium transition and the jamming transition.

[1] D.J. Pine et al., Nature 438, 997(2005).
[2] L. Corté et al., Nature Physics 4, 420 (2008).

DY 17.3 Wed 10:30 H47

A phase field model for platelet-polymer nanocomposit melts — •Thomas Gruhn and Heike Emmerich — MPS, Universität Bayreuth

Nanocomposites of clay nanoplatelets in a polymer matrix combine a high mechanical strength with a low gas permeability so that they can be used, for example, as high quality fire protection materials. The orientational and spatial distributions of the platelets are very important for the materials properties and depend sensitively on the production process. We have developed a novel simulation method for studying the alignment and the density distribution of platelets in the polymer melt. The method combines phase field and liquid crystal theory and allows us to study the dynamics of a system with coexisting domains of high and low platelet concentrations as well as isotropic-nematic phase transitions. The model is used to investigate spinodal decomposition of platelets in the melt. We obtain a new type of spinodal decomposition patterns with an anisotropic structure factor. Results are studied as a function of the platelet concentration.

DY 17.4 Wed 10:45 H47

Density functional theory for hard polyhedra — •Matthieu Marechal[1] and Hartmut Löwen[2] — [1]Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Heinrich Heine Universität Düsseldorf, Düsseldorf, Germany

The ready availability of polyhedral nanoparticles and colloids as a result of recent advances in synthesis methods have allowed experimental observations of crystals of polyhedra. While this realization of polyhedra spurred simulation work on the structure of hard particles, theoretical approaches, so far, have been limited. Using the framework of geometry-based fundamental-measure theory, we develop a classical density functional (DFT) for hard polyhedra and their mixtures. We apply the DFT to Platonic solids (tetrahedra, cubes, octahedra, dodecahedra and icosahedra) and perform Monte Carlo simulations.

Knowledge of the structure of colloids or nanoparticles near a wall is important for understanding heterogeneous nucleation. Furthermore, the density profile near a hard wall provides a standard test case for DFT by comparing with simulation results. The faceted shape of the polyhedra leads to complex layering and orientational ordering near the wall already for a one-component system which is excellently reproduced by our theory. We also considered a 2:1 mixture of tetrahedra and octahedra, which is interesting because it can form a close packed crystal with unit packing fraction. Surprisingly, the local structure in the fluid near the wall for this binary mixture is not similar to the best-packed structure. These effects can be verified in real-space experiments on polyhedral colloids.

DY 17.5 Wed 11:00 H47

Glassy dynamics of Brownian particles close to walls — •Matthias Kohl — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany

By using Brownian dynamics simulations, we study the slowdown of the dynamics of spherical particles at small temperatures or high densities. In our model system, the particles interact via finite-ranged repulsive interactions. In the limit of small overlaps the dynamics of the soft spheres corresponds to the overdamped dynamics of hard spheres. We determine the relaxation time as a function of temperature and pressure. The dynamics in the vicinity of a wall is compared to the dynamics in bulk.

DY 17.6 Wed 11:15 H47

Structure and Dynamics of Suspensions of Colloidal Dumbbells — •Nils Heptner[1,2], Fangfang Chu[1,2], Miriam Siebenbürger[1], Matthias Ballauff[1,2], and Joachim Dzubiella[1,2] — [1]Helmholtz-Zentrum Berlin — [2]Humboldt-Universität zu Berlin, Germany

We investigate the static and dynamic equilibrium structures of a suspensions of colloidal dumbbells by means of Brownian dynamics (BD) computer simulations and linear response theory. These suspension exhibit an elaborate equilibrium phase diagram[1,2]. The particular focus is the study of bulk translational and orientational structure and near-equilibrium transport coefficients at different colloid packing fractions and anisotropy parameters for a better understanding of material properties in and out-of equilibrium.

Crystal structures in the plastic crystal (PC) phase are identified and the PC-liquid transition is investigated. We present structural properties in form of static and dynamic structure factors $S(q, w)$ and pair distribution functions $g(r)$. Furthermore we calculate frequency-dependent rotational and translational self-diffusion constants as well as shear viscosities from equilibrium autocorrelation functions. In addition we will present preliminary results of non-equilibrium simulations imposing oscillatory and steady simple shear flow. All results are compared to the hard sphere reference system as well as available experimental scattering and rheology data.

(1) Vega, C. et al. J Chem Phys 1992, 96, 9060-9072.
(2) Marechal, M.; Dijkstra, M Phys Rev E 2008, 77, 061405.

DY 17.7 Wed 11:30 H47

Polymer statistics in an attractive sphere — Handan Arkin[1,2] and •Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Germany — [2]Department of Physics Engineering, Faculty of Engineering, Ankara University, Turkey

We analyze the structural behavior of a single polymer chain inside an attractive sphere. Our model is composed of a coarse-grained polymer governed by 12-6 Lennard-Jones interactions of the monomers and an attractive sphere potential which follows by integrating the monomer-monomer interaction over the (inner) surface of the sphere. By means

of extensive multicanonical Monte Carlo simulations it is shown that the system exhibits a rich phase diagram in the adsorption strength-temperature ($\epsilon - T$) plane ranging from highly ordered, compact to extended, random coil structures and from desorbed to partially or even completely adsorbed conformations. These findings are identified with different energetic and structural observables including invariant shape parameters such as the asphericity that characterizes the average conformation of the polymer. The resulting phase diagram in the $\epsilon - T$ plane is compared with that for a polymer adsorbing to a plane, attractive substrate obtained previously by Möddel, Bachmann, and one of the authors.

H. Arkın and W. Janke, Phys. Rev. E **85**, 051802 (2012); J. Phys. Chem. B **116**, 10379 (2012); Eur. Phys. J. – Special Topics (in print).

DY 17.8 Wed 11:45 H47

Quantifying shape in heterogeneous media by Minkowski-Tensors — •Michael A. Klatt, Gerd E. Schröder-Turk, and Klaus Mecke — Institut für Theoretische Physik, Universität Erlangen

We describe a novel approach to morphology and anisotropy analysis of complex spatial structure using so-called mixed volumes and Minkowski tensors, which are generalizations of the well-known scalar Minkowski functionals. The tensors are explicitly sensitive to anisotropic aspects of the structure and are relevant for example for elastic moduli or permeabilities of porous materials [1]. A theorem by Alesker (1999) ensures robustness and completeness of a morphological analysis based on Minkowski tensors.

To illustrate the technique we analyze analytically and numerically the spatial structure of the Boolean model of overlapping grains, which is among the most important models for porous and heterogeneous media, leading to good predictions of mechanical and transport properties, e.g., of rock [2]. The morphology of the Boolean model is usually quantified by the mean intercept length for which an analytic expression is presented. However, the commonly used MIL tensor is not well-defined.

An important geometric feature of heterogeneous media is percolation. An accurate estimation of the percolation threshold in Boolean models can be given in terms of mixed volumes and Minkowski tensors.

[1] G. Schröder-Turk et al., Adv. Mater. **23** 2535-2553 (2011).
[2] C. H. Arns et al., Phys. Rev. Lett. **91** 215506 (2003).