DY 55: Posters - Soft Matter, Glasses

Time: Thursday 17:00–19:30   Location: P1A

DY 55.1 Thu 17:00 P1A

Role of surface forces in the spreading of biofilms at solid/gas interfaces — •Sarah Trinschek[1,2], Karin John[2], and Uwe Thiele[1,3] — [1]Westfälische Wilhelms-Universität, Münster, Germany — [2]LiPhy, Université Grenoble Alpes, Grenoble, France — [3]Center for Nonliner Science, Münster, Germany

Biofilms are interface-associated aggregates of bacteria enclosed in a self-produced extracellular matrix. Their widespread occurrence and either detrimental or beneficial function implies that it is highly important to understand the principles underlying their development.

We consider biofilms on moist solid substrates in contact with a gas phase that spread via an osmotic spreading mechanism that is driven by growth processes and the physico-chemical properties of the biofilm and the interfaces. Recent experiments have shown that surface forces are a major determinant of the invasiveness of the colony. We propose a model for the osmotic biofilm spreading that explicitly includes wetting effects. The model is based on a hydrodynamic description for biologically passive liquid suspensions supplemented by bioactive processes. We find a regime where surface forces confine biofilm colonies, which are not able to spread, albeit being biologically active. A small reduction in the surface tension of the biofilm is sufficient to induce lateral spreading of the colony.

DY 55.2 Thu 17:00 P1A

Excitations and defects in colloidal quasicrystals — •Miriam Martinsons and Michael Schmiedeberg — Institut für Theoretische Physik I, FAU Erlangen-Nürnberg, Germany

Quasicrystals are structures with long range order but no translational symmetry. They can have any rotational symmetry including those that are not allowed in periodic crystals. Quasicrystals possess additional degrees of freedom that do not exist in periodic crystals. As a consequence, additional hydrodynamic modes called phasons arise supplemental to the phononic modes known from periodic crystals. Phasonic excitations correspond to correlated rearrangements of the particles.

We study the development of defects close to the melting transition. It has been predicted that dislocations and disclinations cause the melting of the quasicrystal (cf. KTHNY theory [1, 2]). In our studies we reveal the similarities and differences of the melting process of quasicrystals compared to the melting of periodic crystals. Furthermore, we study the influence of phasonic excitations on the formation of defects and their coupling to phononic displacements.

[1] P. De, R. A. Pelcovits, J. Phys. A: Math. Gen. 22, 1167 (1989).
[2] P. De, R. A. Pelcovits, Phys. Rev. B 38, 5042 (1988).

DY 55.3 Thu 17:00 P1A

Supramolecular structure of monohydroxy alcohols at high pressure — Thomas Büning, •Christian Sternemann, Catalin Gainaru, Michael Paulus, Holger Göhring, Susanne Dogan, Julian Schulze, Jennifer Bolle, Roland Böhmer, and Metin Tolan — Fakultät Physik / DELTA, Technische Universität Dortmund, D-44221 Dortmund, Germany

Hydrogen bonds are essential for the structure and dynamics of alcohols, aqueous solutions, and water. Due to their low tendency of crystallization and large variability in molecular configuration, monohydroxy alcohols (MAs) have often been studied as model systems for hydrogen-bonded fluids in general [1]. MAs are supposed to form supramolecular structures via hydrogen bonding in the liquid phase. Tracking the Debye process, dielectric absorption studies suggest ring-like arrangements for 4-methyl-3-heptanol (4M3H) with a sterically hindered hydroxyl group and chainlike structures in 2-ethyl-1-hexanol (2E1H) with the hydroxyl group in a terminal position. Surprisingly, an oppositional behavior of the strength of the Debye process has been observed at increasing pressure for the MAs ponting towards a structural reorganization on the molecular level [2]. We present x-ray diffraction measurements of 2E1H and 4M3H at pressures up to 4500 bar over a temperature range from 273 K to 343 K. The results indicate a breaking of supramolecular structures in both MAs that manifest in significant changes in the first diffraction peak.

[1] R. Böhmer et al., Phys. Reports 545, 125 (2014) and references therein; [2] S. Pawlus et al., J. Chem. Phys. 139, 064501 (2013).

DY 55.4 Thu 17:00 P1A

Phase Field Crystal Models of Colloidal Quasicrystals — •Benedikt Decker and Michael Schmiedeberg — Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Phase field crystal models that employ a Swift-Hohenberg-like free energy are widely used to explore periodic pattern formation [1]. Recently, the phase field crystal model has been modified by adding a second preferred length scale, such that stable quasicrystalline structures are obtained [2,3].

In addition, there are other ways to realize colloidal quasicrystals: A large variety of complex self-organized structures are observed in systems with patchy colloids. Patchy colloids usually carry attractive sites, such that the interaction depends on their orientation. In order to study how such preferred binding angles influence the self-assembly, we construct and explore a phase field crystal model for patchy colloids. Similar to the case of liquid crystals [4], the free energy in such a model depends on order parameters that denote the density as well as the degree and angle of orientation of the particles.

[1] K.R. Elder et al., Phys. Rev. Lett. **88**, 245701 (2002).
[2] J. Rottler et al., J. Phys. Condens. Matter **24**,135002 (2012).
[3] C.V. Achim et al., Phys. Rev. Lett. **112**, 255501 (2014).
[4] C.V. Achim et al., Phys. Rev. E **83**, 061712 (2011).

DY 55.5 Thu 17:00 P1A

Phase behavior of a confined classical Heisenberg fluid — •Stefanie Maria Wandrei[1], Martin Schoen[1,2], and Keith E. Gubbins[2] — [1]Technische Universität, Berlin, Deutschland — [2]North Carolina State University, Raleigh, USA

In this work we employ classical density functional theory (DFT) to investigate equilibrium properties of a Heisenberg fluid confined to nanoscopic slit pores of variable width. Within DFT pair correlations are treated at modified mean-field level. We consider three types of walls: hard ones, where the fluid-wall potential becomes infinite upon molecular contact but vanishes otherwise, and hard walls with superimposed short-range attraction with and without explicit orientation dependence.

If the walls are hard or attractive without specific anchoring the results are "quasi-bulk"-like in that they can be linked to a confinement-induced reduction of the bulk mean field. In these cases the precise nature of the walls is completely irrelevant at coexistence. Only for specific anchoring nontrivial features arise, because then the fluid-wall interaction potential affects the orientation distribution function in a nontrivial way, and thus appears explicitly in the Euler-Lagrange equations to be solved for minima of the grand potential of coexisting phases.

DY 55.6 Thu 17:00 P1A

Low temperature dielectric properties of the polymers poly(vinyl acetate) and poly(vinyl chloride) in the frequency range from Hz to MHz — •Marcel Schrodin, Annina Luck, Benedikt Frey, Lennart Singer, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, 69120 Heidelberg

At low temperatures the behavior of amorphous solids is mainly governed by two level systems and described by the standard tunneling model. In the last years, considerable deviations were observed in dielectric measurements. These deviations are possibly due to the influence of long-range interactions between tunneling systems and the effect of nuclear electric quadrupole moments involved in such tunneling systems.

We show measurements of low temperature dielectric properties of the two amorphous polymers poly(vinyl acetate) and poly(vinyl chloride) in the frequency range from Hz to MHz. As poly(vinyl chloride) contains nuclear electric quadrupole moments due to the presence of the isotopes ^{35}Cl and ^{37}Cl, a possible influence of nuclear quadrupole moments on the dielectric properties can be investigated. In contrast, poly(vinyl acetate) has a similar basic structure but contains only atoms with no nuclear electric quadrupole moment, which enables a direct comparison between both polymers to get a further insight. In addition, both polymers contain large electric dipole moments due to

polar side groups, which allows to look for possible effects of long-range interaction between tunneling systems.

DY 55.7 Thu 17:00 P1A

A lattice system of hard rods in three dimensions — •Axel Gschwind, Martin Oettel, and Miriam Klopotek — Eberhard Karls Universität, Institut für Angewandte Physik, Tübingen

Hard rods in contiuum space with discrete orientations (Zwanzig model) make a useful model for the phase behavior of anisotropic particles, and it was already shown in [1] that these undergo a first-order nematic transition.

For hard rods on a lattice and with discrete orientations one would expect similar behavior. We have studied this system with Grand Canonical Monte Carlo simulations for aspect ratios between 5 and 25. A nematic-isotropic transition is visible starting from aspect ratio 6, but it is only very weakly first order for all aspect ratios investigated. This is in sharp contrast to results from density functional theory for the same system and also from the behavior of hard rods in the continuum.

[1] R. Zwanzig, *First-Order Phase Transition in a Gas of Long Thin Rods*, J. Chem. Phys., **39**(7):1714 (1963).

DY 55.8 Thu 17:00 P1A

From glass to supercooled liquid: long-range correlation of shear strain persists — •Muhammad Hassani and Fathollah Varnik — Interdiciplinary center for advanced material Simulations (ICAMS), Ruhr Universität, Bochum, Germany

While the elasticity in glassy materials is shown to be responsible to mediate long-range strain correlations, there are evidences of similar long-range correlations in the supercooled state as well [1], though low frequency shear modulus vanishes for this state. Via molecular dynamics simulations of a 3D binary Lennard-Jones glass former, we study the temporal evolution of these correlations in supercooled and glassy states [2]. Beside the quadropolar symmetry, the supercooled liquid shares with the glass also the $\frac{1}{r^3}$ power-law decay of strain correlations. Interestingly, the evolution of strain amplitude follows a similar pattern as the single-particle mean-square displacement; in the glass, the amplitude comes to arrest in long time intervals, whereas it follows a diffusive growth in the supercooled state. These findings are in quantitative agreement with the mode-coupling theory predictions which suggest that high viscosity in supercooled state facilitates long-range correlations [3].

[1] J. Chattoraj, A. Lemaître, Elastic Signature of Flow Events in Supercooled Liquids Under Shear, Phys. Rew. Lett.,111, 2013
[2] M. Hassani, F. Varnik, Survey of spatio-temporal strain correlations across the glass transition, (in preparation)
[3] B. Illing, S. Fritschi, D. Hajnal, C. Klix, P. Keim,M. Fuchs, Strain Pattern in Supercooled Liquids, Phys. Rev. Lett. 117, 208002

DY 55.9 Thu 17:00 P1A

Theory for the activation energy in mixed glass former glasses — •Mohamad Alhamad and Philipp Maass — Universität Osnabrück, Fachbereich Physik, Barbarastraße 7, 49076 Osnabrück, Germany

Improved physical and electrochemical properties of glassy electrolytes can be achieved by mixing two glass former cat- or anions at constant mole fraction of the mobile cation. This effect is known as the mixed glass former effect. Optimized mixed glass former electrolytes are promising materials for developing next generation solid state batteries. Most important is the optimization of the ionic conductivity and its activation energy. Extending a previous approach [1], we present a theory that allows us to predict the dependence of the activation energy on the glass former mixing ratio based on the charge redistribution in the glassy network. This redistribution is caused by changes in the concentration of the various network forming units associated with the glass formers. The latter are modeled within a thermodynamic model and the resulting change of the activation energy by applying percolation theory. Application of the theory leads to excellent quantitative agreement with measurements for five different types of alkali conducting mixed glass former systems with mixing pairs B_2O_3/P_2O_5, $GeS_2/PO_{5/2}$, B_2O_3/Si_2O_4, B_2O_3/TeO_2, and $PO_{5/2}/TeO_2$.

[1] M. Schuch, C. Trott, P. Maass, RSC Adv. **1**, 1370 (2011).

DY 55.10 Thu 17:00 P1A

Irreversibility transition of colloidal polycrystals under cyclic deformation — •Pritam Kumar Jana[1], Mikko J. Alava[1], and Stefano Zapperi[1,2,3,4] — [1]COMP Centre of Excellence, Department of Applied physics, Aalto University, P.O. Box 11100, Aalto 00076, Finland — [2]Center for Complexity and Biosystems, Department of Physics, University of Milano, via Celoria 16, 20133 Milano, Italy — [3]ISI Foundation, Via Alassio 11/C, 10126 Torino, Italy — [4]CNR-IENI, Via R. Cozzi 53, 20125 Milano, Italy

Recently, Tamborini et al. have investigated plasticity of colloidal polycrystals, which are prepared by crystallizing thermo sensitive block copolymer Pluronics F108 with a small amount of nanoparticles as impurities, under cyclic shear. [1] Guided by their experiment, we perform plastic deformation study on 2D polycrystalline samples using molecular dynamics simulations. Samples are prepared by reducing the temperature of binary Lennard-Jones liquids with a fixed cooling rate. A small amount of bigger particles, which basically acts as an impurity, creates dislocations in the system because of size mismatch. A string of dislocations are defined as grain boundaries and the amount of impurities can control the number of grains. In the next stage, samples are undergone a cyclic deformation where the maximum strain amplitude (γmax) is varied by changing the strain rate. For a small value of γmax, the system becomes quiescent within a few cycles whereas for larger γmax, particles move irreversibly which leads to the grain boundary motion and the annihilation of dislocations.

[1] Tamborini et al. PRL 113, 078301 (2014)

DY 55.11 Thu 17:00 P1A

Aging and Coarsening During Polymer Collapse — •Suman Majumder and Wolfhard Janke — Institute for Theoretical Physics

Using state of the art Monte Carlo simulations of a bead-spring model we investigate both the equilibrium and the nonequilibrium behavior of a homopolymer collapse. The equilibrium properties obtained via multicanonical sampling recover the well-known finite-size scaling behavior of collapse for our model polymer. For the nonequilibrium dynamics we study the collapse by quenching the homopolymer from an expanded coiled state into the globular phase. The sequence of events observed during the collapse is independent of the quenched depth. In particular, we focus on finding out universal scaling behaviors related to the growth or coarsening of clusters of monomers, by drawing phenomenological analogies with ordering kinetics. We distinguish the cluster growth from the initial nucleation stage and show via nonequilibrium finite-size scaling analyses that the clusters grow linearly at all temperatures. In addition, we provide evidence of aging by constructing a suitable autocorrelation function and its corresponding dynamical power-law scaling with respect to the growing cluster sizes. The predicted theoretical bound for the exponent governing such scaling is strictly obeyed by the numerical data irrespective of the quench temperature. The results and methods presented here in general should find application in similar phenomena such as the collapse of a protein molecule preceding its folding.

DY 55.12 Thu 17:00 P1A

Induced anomalous diffusion nearby elastic interfaces — •Abdallah Daddi-Moussa-Ider, Achim Guckenberger, and Stephan Gekle — Biofluid Simulation and Modeling, Universität Bayreuth, Universitätsstraße 30, Bayreuth 95440, Germany

The approach of a small particle to the cell membrane represents the crucial step before active internalization and is governed by thermal diffusion. Using a fully analytical theory, we show that the membrane induces a long-lived subdiffusive behavior on the nearby particle, during which the residence time is increased by up to 50 % for a typical scenario. The corresponding scaling exponent is found to be as low as 0.87 in the perpendicular direction, and as low as 0.92 in the parallel direction. Such behavior is qualitatively different from the normal diffusion near a hard wall or in a bulk fluid. A good agreement is found for the frequency dependent mobility between the analytical predictions and the numerical simulations that we performed using a boundary integral method.

References
[1] Daddi-Moussa-Ider, A., Guckenberger, A. and Gekle, S., Phys. Rev. E 93, 012612 (2016)
[2] Daddi-Moussa-Ider, A., Guckenberger, A. and Gekle, S., Phys. Fluids 28, 071903 (2016)