CPP 5 SYMPOSIUM: Dynamics of multi-component fluids POSTER

Zeit: Freitag 17:15–19:00 Raum: Poster TU D

CPP 5.1 Fr 17:15 Poster TU D

Flow electrification in non-aqueous colloidal suspensions, studied with video microscopy — •Michael Duits, Valentin Tolpekin, Dirk van den Ende, and Jorrit Mellema — University of Twente

We observed flow electrification in concentrated binary suspensions of hydrophobized silica particles in chloroform. In this low polarity solvent, electrical charges on the large-particles surfaces manifest themselves via long-ranged forces. On shearing the suspension for prolonged time, the interactions between large particles were found to change from weakly attractive (due to the small particles) to strongly repulsive (due to acquired Coulomb interactions). A spectacular manifestation of the phenomenon was observed with video microscopy. After an initial aggregation stage, disintegration into mostly primary particles occurred. The flow electrification was further corroborated by control experiments, without flow or with antistatic agent: here the aggregates kept on growing. We also did experiments where an electric field was applied to the suspension. A similarity was found with the original experiment, suggesting that herein the glass wall acquired negative charges. Aggregates also disintegrated in electric fields, but now the result was a segregated fluid: a coexistence of regions enriched in large particles, and regions depleted of them. At rest these regions exist as isolated units, but in shear flow they merge into bands, a behavior which resembles shear banding.

CPP 5.2 Fr 17:15 Poster TU D

Structure in systems of chemically heterogeneous colloidal rods — •Thomas Gruhn, Chelakkot Raghunath, and Reinhard Lipowsky — MPIKG Golm, D-14424 Potsdam, Germany

Colloidal rod-like macromolecules like cylindrical dendrimeres can nowadays be synthesized in large amounts. The length scale of the rods allows tailored chemical structuring of the rods. We performed Monte Carlo simulations of systems of chemically structured rods whose interaction potential varies along the rod axis. We have focussed on repulsive, hard rods with short-range attractive end groups. For higher pressures they behave qualitatively similar to hard rods. At low pressure the system forms complex, scaffold-like network structures. Qualitative features and the stability of the self-assembled structures can be modified by introducing an angular dependence of the attractive end groups.

Chemically heterogeneous rods turn out to be excellent building blocks for super-porous, self-assembling materials. With a mixture of different rods an even larger class of structures can be achieved.

CPP 5.3 Fr 17:15 Poster TU D

Dynamic density functional theory for interacting Brownian particles: deterministic or stochastic? — •Markus Rauscher[1,2] and Andrew J. Archer[3] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart, Germany — [2]ITAP, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart,Germany — [3]H. H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, UK

Dynamic density functional theory (DFT) is a dynamic extension of the very successful equilibrium DFT to systems close to equilibrium. For example, dynamic DFT has been used to describe non-equilibrium entropic interactions between colloids in polymer solutions. There has been a confusions in the literature as to whether or not dynamic DFT for the one-body density of a classical Brownian fluid should contain a stochastic noise term. We aim to clarify this confusions by revisiting the derivations of DDFT and point out that a stochastic as well as a deterministic equation of motion for the density distribution can be justified, depending on how the fluid one-body density is defined – i.e. whether it is an ensemble averaged density distribution or a spatially and/or temporally coarse grained density distribution [1].

[1] A. J. Archer and M. Rauscher, J. Phys. A: Math. General **37**, 9325 (2004)

CPP 5.4 Fr 17:15 Poster TU D

— •Christian Holm, Burkhard Dünweg, and Vladimir Lobaskin — Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz

We study the mobility of a charged colloidal particle in a constant homogeneous electric field by means of computer simulations. The simulation method combines a lattice Boltzmann scheme for the fluid with standard Langevin dynamics for the colloidal particle, which is built up from a net of bonded particles forming the surface of the colloid. The coupling between the two subsystems is introduced via friction forces. In addition explicit counterions, also coupled to the fluid, are present. We observe a non-monotonous dependence of the electrophoretic mobility on the bare colloidal charge. At low surface charge density we observe a linear increase of the mobility with bare charge, whereas at higher charges, where more than half of the ions are co-moving with the colloid, the mobility decreases with increasing bare charge.

[1] V. Lobaskin, B. Dünweg, C. Holm, *Electrophoretic mobility of a charged colloidal particle: A computer simulation study*, J. Phys.: Condens. Matter **16** S4063-S4073 (2004)

CPP 5.5 Fr 17:15 Poster TU D

Hydrodynamic simulation of star polymers under shear — •Marisol Ripoll, Kiaresch Mussawisade , Roland G. Winkler, and Gerhard Gompper — IFF, Forschungszentrum Juelich, Germany

The dynamics of star polymers in solution under shear flow is studied through a novel mesoscopic simulation technique called Stochastic Rotation Dynamics (SRD) or alternatively Multi-Particle-Collision dynamics (MPCD) [1]. It has been demonstrated that, by varing the model parameters, the Schmidt number can be large enough such that the solvent properly accounts for hydrodynamic interactions [2].

In this work, the influence of shear on a single star polymer is analyzed as a function of the shear rate, the functionality of the star, the length of the arms, and the properties of the solvent. It is observed that for shear rates exceeding the rotational relaxation time of a single arm, the star polymer deforms and aligns with the shear flow.

[1] A. Malevanets and R. Kapral. *J. Chem. Phys*, **110**, 8605–8613, (1999). *J. Chem. Phys*, **112**, 7260–7269, (2000).

[2] M. Ripoll, K. Mussavisade, R. G. Winkler and G. Gompper. *Europhys. Lett.*, **68**, 106–112, (2004). R. G. Winkler, K. Mussavisade, M. Ripoll and G. Gompper. *J. Phys.:Condens. Matter*, **16**, S3941–S3954, (2004).

CPP 5.6 Fr 17:15 Poster TU D

Liquid to solid transition of inverse ferrofluids — •Ruben Saldivar-Guerrero[1,2], Reinhard Richter[1], Ingo Rehberg[1], Nuri Aksel[3], Lutz Heymann[3], and Oliverio S. Rodriguez-Fernandez[2] — [1]Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth, Germany — [2]Centro de Investigacion en Quimica aplicada, 25100 Saltillo, Mexico — [3]Technische Mechanik und Strömungsmechanik, Universität Bayreuth, D-95440 Bayreuth, Germany

By disperging microsized polystyrene particles in ferrofluid an ideal magneto-rheological model fluid can be created. Because polystyrene particles are available, which are practically monodisperse ($\sigma = 0.04$), this hybrid fluid allows to controll particle size and polydispersity, in advantage to the common ferro- and magneto-rheological fluids, which are only polydisperse. The nonmagnetic polystyrene particles create a hole in the ferrofluid, which appear to posses a magnetic moment corresponding to the amount and suszeptibility of the displaced fluid. Due to the dipolar interactions of the holes chain formation sets in and the inverse fluid undergoes a transition from liquid to solid like behaviour. We investigate this transition by recording the storage modulus G' and the loss modulus G" versus the magnetic field for different volume fraction, particle size, and particle size distribution. Our results show that for a monodisperse fluid the liquid to solid transition is more pronounced than for a polydisperse one - a related effect has recently been found in MD simulations for standard ferrofluids (Z. Wang , and Ch. Hol, Phys. Rev. E 2003).

CPP 5.7 Fr 17:15 Poster TU D

Transport of Liposomes through Pores — •Gunnar T. Linke, Thomas Gruhn, and Reinhard Lipowsky — Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, D-14776 Golm, Germany

In the last decade, liposomes have become an important drug delivery system. One important application is the transport of anti-tumor drugs into the affected tissue. As found in experiments, the endothelium of blood vessels in cancer tissues is irregularly formed and contains large gaps, which allow an increased uptake of liposomes. Another application of liposomes is the osmotically induced transcutaneous transport of encapsulated substances through narrow pores in the skin.

Free energy barriers for these transport processes are estimated by means of Monte Carlo simulations. In case of narrow pores, the free energy barrier may vanish for liposomes with a second component which has a positive spontaneous curvature. Further, it is shown that a homogeneous spontaneous curvature drastically reduces the free energy barrier for the transport of liposomes through pores with radii slightly smaller than the liposome radius.

CPP 5.8 Fr 17:15 Poster TU D

Slow Relaxation Dynamics of Tubular Polymersomes after Thermal Quench — •Antje Adriana Reinecke[1] and Hans-Günther Döbereiner[2] — [1]Max-Planck-Institut für Kolloid- und Grenzflächenforschung, D-14424 Potsdam — [2]Department of Biology, Columbia University, New York, NY 10027

Morphological shape changes of giant tubular vesicles prepared from the diblock copolymer polybutadiene- (32)-b-polyethylene oxide(20) (PB-PEO) in aqueous solution after thermal quenches between 10 and 50K were monitored via quantitative phase-contrast microscopy [1]. Reducing the temperature leads to extremely slow sequential beading of the tubes where the formation of necks starts symmetrically at the two ends. We characterize the neck diameters and find that the necks close one by one with effective velocities on the order of a few tens of nanometers per minute. The necks do not close continuously, but rather their radii decrease in time in a sequence of exponential decays between intermediate plateaus. The slow dynamics is a result of the high membrane surface viscosity of PB-PEO. Sequential beading is rationalized via a cascade of metastable shapes determined by the bending elastic energy of the tubular polymersomes.

[1] A. Reinecke, H.-G. Döbereiner, Langmuir 19, 605-608 (2003)

CPP 5.9 Fr 17:15 Poster TU D

Adhesion control of membranes by active stickers — •Bartosz Rozycki[1,2], Reinhard Lipowsky[2], and Thomas R. Weikl[2] — [1]Instytut Fizyki Teoretycznej, Uniwersytet Warszawaki, 00-681 Warszawa, Hoza 69, Poland — [2]Max-Planck-Institut fur Kolloid- und Grenzflachenforschung, 14424 Potsdam, Germany

Biological membranes actively control their adhesion states. We consider here a simple theoretical model of membranes with active adhesion molecules, or ‘stickers’. The stickers are actively switched ‘on’ or ‘off’, which keeps the system out of thermal equilibrium. We find that the phase behavior of the membranes depends rather sensitively on the switching rates of the stickers, and not only on the fraction of ‘on’-stickers. In the asymptotic regimes of ‘slow’ and ‘fast’ switching, we obtain exact results which relate the unbinding behavior of the active membranes to well-studied properties of equilibrium membranes. Using Monte Carlo simulations, we show that the characteristic crossover time scale between the asymptotic regimes is given by the binding time of the stickers. Our results may provide insights into novel mechanisms for the controlled adhesion of biological or biomimetic membranes.

CPP 5.10 Fr 17:15 Poster TU D

Diffusion and encapsulation of dextran probe molecules in sub-micron polyelectrolyte capsule dispersions measured using PFG-NMR — •Monika Schönhoff[1] and Thorsteinn Adalsteinsson[1,2] — [1]Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, D-48149 Münster — [2]current address: Department of Chemistry, Mount Holyoke College, S. Hadley, MA 01075, U.S.A.

Pulsed field gradient NMR(PFG-NMR) is introduced to probe the distribution and dynamics of long dextran sugars in colloidal dispersions of sub micron hollow polymeric capsules. The capsules are prepared using the layer-by-layer (LBL) self assembly method of strong polyelectrolytes onto silica particles, followed by a dissolution of the silica core. The capsules are permeable for water and small ions, but large molecules, such as polydextran, are found to be in slow exchange between two sites, the capsule interior and the exterior. 1H spin-spin (T2) and spin-lattice (T1) relaxation times of the encapsulated dextran are estimated from combined diffusion-relaxation measurements. Both relaxation times are used to calculate the population of encapsulated dextran and to discuss the state of the encapsulated dextran. The NMR measurements here indicate that the dextran may preferentially select the capsule interior, resulting in an enriched dextran concentration inside the capsules. The encapsulated dextran appears to be in a liquid-like state rather than being immobilized on the capsule wall. [J. Phys. Chem. B, in press]

CPP 5.11 Fr 17:15 Poster TU D

Capillary breakup of complex liquids and the elongational viscosity — •Christian Wagner — Experimentalphysik, Universitaet des Saarlandes, 66123 Saarbruecken

The detachment process of a droplet of an elastic liquid is characterized by the suppression of the pinch off finite time singularity and the formation of a cylindrical filament between the droplet and the nozzle. The flow in this filament is purely elongational. The resistance to such a flow is macroscopically described by the elongational viscosity. However, a sound understanding of the functional connection between the microscopic configurations of the polymer molecules and the macroscopic flow is still missing. We present birefringence data that are taken simultaneously to the macroscopic flow measurements. By changing the ionic strength of the solvent we can tune the flexibility of our polyelectrolytic macromolecules and correlate them with the microscopic polymer configurations and the measurements of the elongational viscosity.

CPP 5.12 Fr 17:15 Poster TU D

Buckling Instability of Droplet Chains in Liquid Crystalline Films — •Camilla Völtz and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg, D-39106 Magdeburg, Germany

Isotropic droplets on smectic films present a model for two-dimensional colloids. A characteristic feature of the droplets is their mutual interaction by elastic distortions of the local orientation of the film, the *c*-director. We focus on the experimental investigation of the spontaneous deformation of droplet structures (buckling).

Under certain conditions, the *c*-director field in a free-standing smectic film can be prepared in such a way, that it is continuously rotated and forms a target pattern. Droplets are induced in the photochromic material by variation of the illumination strength. They align in closed chain rings. Increment of the droplet number increases the chain length at constant ring diameter, leading to a buckling instability with spontaneous wavelength selection.

CPP 5.13 Fr 17:15 Poster TU D

Phase-separation by evaporating polymer blend solution subjected to flow
— •P. Müller-Buschbaum[1], E. Bauer[1], S. Pfister[1], S.V. Roth[2], M. Burghammer[2], C. Riekel[2], U. Thiele[3], and C. David[4] — [1]TU München, Physik-Department E13, James-Franck-Str. 1, D-85747 Garching, Germany — [2]ESRF, BP 220, 38043 Grenoble Cedex 09, France — [3]MPI f. Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany — [4]Laboratory for Micro- and Nanotechnology, PSI, CH-5232 Villigen, Switzerland

Multiscale polymeric patterns resulting from flow of a binary polymer blend solution of polystyrene and poly-n-buthylacrylate in toluene on an inclined substrate are analysed with sub-microbeam GISAXS [1] and real space techniques. The locally isotropic phase-separation structure on the 1 micron level is embedded in a super structure on the 100 micron level of stripe-like variations of film thickness *and* composition oriented perpendicular to the flow direction. The multiscale pattern result from the interplay of evaporation, convective flow, diffusion and spinodal decomposition.

[1] P.Müller-Buschbaum, S.V.Roth, M.Burghammer, E.Bauer, S.Pfister, C.David, C.Riekel, Physica B at press

CPP 5.14 Fr 17:15 Poster TU D

Monodisperse Emulsions Confined to Channels — •Magdalena Ulmeanu, Dmytro Melenevsky, Stephan Herminghaus, and Ralf Seemann — MPI for Dynamics and Self-Organization, D-37073 Göttingen

The controlled manipulation of liquid compartments within microchannels has been termed digital microfluidics. The crucial issue here is the interplay of the size of the liquid compartments, with the lateral dimension of the channels. This enables comprehensive control of microfluidic processing like sorting, mixing, reacting, separating, provided all liquid compartments are equally sized. Emulsion droplets with diameter in between 2 and 20 microns provide suitable compartments for very small quantities of solvents or reagents. We therefore study several techniques for the preparation of highly stable and monodisperse microemulsions. Subsequent to the preparation, the continuous phase of the emulsion is reduced. The resulting gel emulsion is analogous to a dry foam, why we tend to term it spumo-emulsion (lat. spuma = foam). It exhibits a variety of transitions in its topology upon interaction with an externally provided (temporally variable) geometric constraint. We exploit the interaction of the internal length scale of these compartmented fluids with the lateral dimension of micro channels. In addition, we study the formation of 2D and 3D emulsion crystals by mixing droplets with two distinct diameters with a certain size ratio, which may lead to a novel type of chemical reaction setup and new materials.

CPP 5.15 Fr 17:15 Poster TU D

Relaxation and recovery phenomena in melts of PS/PMMA blends — •Ulrich A. Handge — Institute of Polymers, Department of Materials, ETH Zürich, HCI H 529, Wolfgang-Pauli-Straße 10, 8093 Zürich, Switzerland

The rheological properties of melts of binary blends of immiscible polymers are strongly influenced by the viscoelastic properties of the single components and the interfacial tension between the two phases. The interfacial tension contributes to the viscoelasticity of the molten blend. In this work, we focus on interfacial tension driven relaxation and recovery phenomena in a molten polystyrene/poly(methyl methacrylate) (PS/PMMA) blend and report on experimental phenomena and theoretical models. In relaxation after melt elongation, the interfacial tension can cause interesting breakup phenomena, for example undulations of the Rayleigh instability [1] and formation of holes and fingers in equibiaxially highly elongated PS droplets [2]. These breakup phenomena play a key role for polymer processing. In recovery experiments, the interfacial tension increases the elasticity of the melt, an effect which can be theoretically described by an effective medium approximation [3-5].
[1] S. Tomotika, *Proc. Roy. Soc. Lond. Ser. A* **150**, 322 (1935).
[2] U.A. Handge, in preparation.
[3] U.A. Handge, *J. Rheol.* **47**, 969 (2003).
[4] U.A. Handge, *AIP Conference Proceedings* **708**, 52 (2004).
[5] U.A. Handge and P. Pötschke, *J. Rheol.* **48**, 1103 (2004).

CPP 5.16 Fr 17:15 Poster TU D

Correlation between Morphology and Rheology of Mica-Filled Polyethylene — •Albrecht Kuelpmann, Maged A. Osman, and Ulrich W. Suter — ETH Zurich, Institute of Polymers, 8093 Zurich, Switzerland

This contribution deals with the rheological behavior of mica-filled HDPE melts and its correlation to the microstructure of the composites. A method was developed to measure in-plane and out-of-plane shear properties of these transversely isotropic composites experimentally. To describe the microstructure of the composites, the size and aspect ratio distribution of the dispersed platelets were determined from SEM micrographs by image analysis. The orientation of the particles was obtained from X-ray rocking curve measurements. The elastic reinforcement by the platelets was described by the Halpin-Tsai equation and yielded a reinforcement parameter as a function of the aspect ratio and the orientation. At low shear frequencies, the relative storage modulus exhibited a frequency dependence with increasing filler loading. Relaxation time spectra revealed that these viscoelastic effects were due to an increased relaxation strength at long relaxation times. The extend of these viscoelastic effects scaled with the volume specific surface area rather than size or aspect ratio of the particles. These findings supported a bridging mechanism between particles by polymer.

CPP 5.17 Fr 17:15 Poster TU D

Estimating the molecular weight distribution of polymer melts from viscoelastic responds — •Andreas W. Liehr, Philippe-André Bourdin, and Christian Friedrich — Material Research Center Freiburg, Stefan-Meier-Str. 21, D-79104 Freiburg i. Br.,Germany

Fast and easy accessible methods for the estimation of the molecular weight distribution of polymer melts is an important issue of modern polymer physics. In this talk we discuss approaches basing on measured linear viscoelastic properties of the samples. Applying advanced models [1] describing the interrelation between molecular structure and viscoelastic properties we are able to focus on the solution of the inverse problem. Starting point is a contour length fluctuation model with Rouse modes, which predicts the relaxation modulus of a polymer melt from its molecular weight distribution. The inverse problem resulting from this model is solved by a nonlinear regularization method [2].
[1] van Ruymbeke, E. ; Keunings, R. ; Stéphenne, V. ; Hagenaars, A. ; Bailly, C.: Evaluation of Reptation Models for Predicting the Linear Viscoelastic Properties of Entangled Linear Polymers. In: *Macromolecules* 35 (2002), S. 2689–2699
[2] Honerkamp, J. ; Weese, J.: Determination of the Relaxation Spectrum by a Regularization Method. In: *Macromolecules* 22 (1988), Nr. 11, S. 4372–4377

CPP 5.18 Fr 17:15 Poster TU D

Kinetics of ternary polymer blend films investigated with neutron reflectometry and AFM — •P. Panagiotou[1], E. Maurer[1], R. Cubitt[2], and P. Müller-Buschbaum[1] — [1]TU München Physik Department LS E13, James-Franck-Str. 1, 85747 Garching (Germany) — [2]ILL D17, rue Jules Horowitz 1, BP 156 - 38042 Grenoble Cedex 9 - (France)

By blending polymers with different properties in terms of their molecular weight, glass transition temperature and ratio of mixture immiscible new structures are observable. In the present investigation three different polymer components were solved at a given mass concentration in toluene and blended at a specified weight fraction. This polymer solution was spin-coated onto a pre-cleaned Si(100) wafer. By further preparation based on annealing and swelling in solvent vapor the morphology was under kinetic transformations. These kinetic changes of the system have been investigated in-situ with neutron reflectometry (D17 at ILL). With its horizontal plane scattering geometry set-up and its time-of-flight (TOF) mode detection of the specular signal a high time resolution of 60 sec was achieved. During the swelling process the polymer film undergoes a phase separation. The deuterated component diffuses from the substrate towards the surface, while the total thickness of the blend film increases due to the embedded solvent molecules. As three different swelling temperature were investigated the kinetic process was tuned.

CPP 5.19 Fr 17:15 Poster TU D

Interface velocity of a structured liquid on solid substrates: a SPM study — •Daniel Podzimek and Karin Jacobs — FR 7.2 Experimental Physics - Soft Matter, Saarland University, D-66123 Saarbrücken

We report novel experiments that enable a direct insight into the flow properties of thin liquid films. The flow properties have been evaluated for liquid fronts that move over solid substrates, driven by interfacial forces arising from the films being deposited onto non-wetting substrates. The dewetting process involves the nucleation and growth of holes induced by heating polymer films above their glass transition temperature. Our experiments are performed on the moving liquid fronts surrounding those holes using a thin block copolymer film as a structured liquid. Since the two blocks of the poly(styrene-ethylene/propylene) copolymer are incompatible, they phase separate and microdomains emerge. Upon shear (induced by dewetting), these microdomains undergo a structural rearrangement and form cylinders. We report first direct SPM experiments on the liquid/solid interface with nanometer resolution. At this interface we find a similar microdomain alignment as on top of the film. This alignment, which is due to a nonzero slippage velocity at the interface, gives us a powerful tool to investigate the slippage length of melts of different viscosities on different substrates.

CPP 5.20 Fr 17:15 Poster TU D

Dynamical Model for Chemically Driven Running Droplets — •Uwe Thiele[1], Karin John[1], and Markus Bär[1,2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany — [2]Physikalisch-Technische Bundesanstalt, Abbestrasse 2 - 12, D-10587 Berlin, Germany

Chemically driven self-propelled running droplets are studied employing dynamical models [1]. We use coupled evolution equations for the film thickness profile and the adsorbate coverage of the solid substrate. The film evolution equation includes a disjoining pressure that models the adsorbate dependent wettability. In the adsorbate evolution equation we employ different reaction terms that (a) only allows for adsorption underneath the droplet [1] or (b) allows furthermore for desorption at the 'bare' substrate. The two models describe different sets of experiments found in the literature [2-4]. Change of the reaction rate or maximal wettability difference allows for qualitatively different regimes of the drop movement corresponding to experimental results [2,3]. Finally, we discuss a model for running droplets whose movement is caused by an ongoing phase transition.

[1] U. Thiele, K. John and M. Bär, *Phys. Rev. Lett.*, **93**, 027802 (2004); [2] F. Domingues Dos Santos and T. Ondarcuhu, *Phys. Rev. Lett.* **75**, 2972 (1995); [3] S. W. Lee, D. Y. Kwok, and P. E. Laibinis, *Phys. Rev. E* **65**, 051602 (2002); [4] Y. Sumino *et al.*, to be published (2004).

CPP 5.21 Fr 17:15 Poster TU D

Running droplets through chemical decomposition of block copolymers in thin films — •Stephan Weiss, Andriana Horvat, Armin Knoll, Larissa Tsarkova, and Robert Magerle — Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth

We investigate 30-100 nm thin films of poly(styrene)-*block*-poly(ethylenepropylene) (PS-PEP). Upon annealing in air (in the range of 130-190 °C) the microdomain structure coarsens and forms ~ 0.3 μm large PS domains embedded in a PEP matrix. When two PS domains coalesce, the resulting domain starts to move spontaneously across the surface and grows to a macroscopic droplet. Behind the droplet a $\sim$10 nm thick film is left. The phenomenon is followed with tapping mode scanning force microscopy and optical microscopy. We show that a chemical reaction with oxygen is essential for droplet motion. We study the influence of film thickness, annealing temperature, and atmosphere on the kinetics of the phenomenon. Similarities and differences to other reactive wetting phenomena are discussed.

CPP 5.22 Fr 17:15 Poster TU D

Structural changes in diblock-copolymer micelles induced by comicellization with surfactants — •Thomas Hellweg[1], Anette Nordskog[1], and Helmut Schlaad[2] — [1]TU Berlin, Stranski-Laboratorium, Strasse des 17.Juni 112, 10623 Berlin — [2]MPI-KGF, Potsdam-Golm, 14424 Potsdam

Because of the incompatibility of the two blocks of amphiphilic block-copolymers, they form micellar aggregates in selective solvents. In the present work we investigate the influence of ionic surfactants on the structure of nonionic diblock-copolymer micelles applying the concept of changing the natural curvature of amphiphilic interfaces, which allows to tune the micellar shape. The diblock-copolymer polybutadien-b-poly(ethyleneoxide) PB-PEO with a ratio of the block sizes $N_{PB}/N_{PEO} \geq 3/4$ forms wormlike micelles in aqueous solutions [1]. Upon addition of short-chain ionic surfactants mixed block-copolymer/surfactant micelles are formed. Because of the repulsive interactions of the ionic headgroups the effective headgroup area increases, which leads to a higher curvature of the amphiphilic interface and a change of the overall micellar structure. Using mainly static and dynamic scattering techniques the influence of different surfactants on these block-copolymer micelles is investigated [1, 2].

[1]A. Nordskog, H. Egger, G. H. Findenegg, Th. Hellweg, H. Schlaad, H. von Berlepsch, and C. Böttcher: Phys. Rev E, 68 (2003) 11406/1-14. [2]A. Nordskog, T. Fütterer, H. Schlaad, A. Heinemann, H. von Berlepsch, C. Böttcher, and Th. Hellweg: PCCP, 6 (2004) 3123-3129.

CPP 5.23 Fr 17:15 Poster TU D

Modification of forces in aqueous wetting nanofilms — •Katarzyna Ciunel[1] and Regine v. Klitzing[2,3] — [1]Stranski-Laboratorium, TU Berlin — [2]MPI f. Kolloid- und Grenzflächenforschung, Potsdam — [3]Institut f. Physikalische Chemie, CAU Kiel

Thin liquid films are the building blocks of many macroscopic systems (e.g. foams, emulsions), and they affect the stability and functions of these systems. The forces between the opposing interfaces depend on the composition of the film interfaces and of the film fluid. The sum of interactions between the film surfaces is determined quantitatively by the disjoining pressure isotherm (disjoining pressure in dependence vs. film thickness) and it is measured by varying the outer pressure in a so-called thin film pressure balance. The approach of a solid substrate to one of the film interfaces (wetting film) changes the drainage behaviour with respect to a free-standing film. The opposing air/water interface is varied by the adsorption of different amphiphiles. In order to modify the interactions between the fluid and the interface, the solid surface is pre-coated by polyelectrolytes of different charge. The factors dominating the stability are figured out by static and drainage measurements.

CPP 5.24 Fr 17:15 Poster TU D

THE MOLECULAR ORIGIN OF FOAM STABILITY: A VIBRATIONAL SURFACE SUM FREQUENCY STUDY OF THE INTERFACIAL WATER — •Patrick Koelsch and Hubert Motschmann — Max-Planck-Institute of Colloids and Interfaces, Am Muehlenberg, 14476 Potsdam, Germany

Foam formation and foam stability must be clearly distinguished. While foam formation could successfully be linked to the relative dynamic surface pressure, it turned out to be impossible to establish a similar relation between foam stability and a fundamental system parameter.

A novel measurement technique developed at the MPI-KGF allows precise measurement of the complex surface dilatational modulus in a broad frequency range. These measurements clearly relate the intrinsic surface dilatational viscosity to the stability of a foam lamella. The intrinsic surface viscosity damps film deformation prior to bubble rupture.

However, what is the molecular process which dissipates the energy? To study this, we performed Infrared Visible Sum Frequency Generation Spectra of two surfactant systems, one forming stable foam lamellas and the other not. The surface tension and magnitude of the elasticity modulus is comparable in both cases. IR-VIS SFG spectrum records the vibronic signature of the surface layer with a high surface specificity. The interfacial water structure shows in both cases striking differences. A molecular picture of the dissipative process is derived.

CPP 5.25 Fr 17:15 Poster TU D

Coarse-Graining of non-bonded molecules? — •Sabine H.L. Klapp[1], Henry Bock[2], and Keith E Gubbins[2] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Sekr. TC7, Technische Universität Berlin, Strasse des 17. Juni 124, 10623 Berlin, Germany — [2]Department of Chemical Engineering, North Carolina State University, 113 Riddick Labs, Raleigh, NC 27695-7905, USA

In coarse–grained ("mesoscale") computer simulations of complex mixtures, such as surfactants in aqueous solution, two routes are generally followed: the first route consists of considering only the motion of the surfactant molecules and integrating out the water completely. The water is then treated only implicitly via the effective potential between surfactants. The other possibility, which is the one commonly used in Dissipative particle dynamics (DPD) simulations, is to keep explicit "beads"containing several *non–bonded* water molecules. In this contribution we demonstrate, based on exact expressions for effective potentials, that coarse–graining of non–bonded molecules such as water does not work in the sense that the corresponding effective potential vanishes.

CPP 5.26 Fr 17:15 Poster TU D

Domain Formation from Dissipative Particle Dynamics — •Gregoria Illya — MPI Colloids and Interfaces, D 14424, Potsdam, Germany

Dissipative Particle Dynamics is used to simulate the formation of domains in two-component vesicles whose constituent molecules differ in their architecutre and interactions. The domains can be circular, stripe-like, or form more complex arrangements, depending on the vesicle composition and the molecular architectures.

CPP 5.27 Fr 17:15 Poster TU D

Magnetic Field Induced Orientation in Diblock Copolymers with One Crystallizable Block — •T. Grigorova[1], S. Pispas[2], T. Thurn-Albrecht[1], and N. Hadjichristidis[2] — [1]FB Physik, Martin-Luther Universität Halle-Wittenberg, 06120 Halle (Saale), Germany — [2]Department of Chemistry, University of Athens, 15784 Ilissia, Greece

Crystallization of semicrystalline polymers in a strong magnetic field under appropriate thermal conditions leads to the formation of an oriented texture. We have applied that effect to induce orientation in semicrystalline block copolymers and show that asymmetric PEO-b-PB copolymers can be easily aligned if the crystallization starts from a disordered state. Necessary condition is that the crystallization starts from a high number of nuclei. The magnetic field can induce orientation only during the initial stage of the spherulitic growth before branching of crystallites takes place. The orientation of the crystallites, observed with wide angle X-ray scattering, goes along with the orientation of the block copolymer microphase structure. The resulting lamellar structure is oriented with the lamellar normal parallel to the direction of the applied field (negative order parameter), similarly as for electric field induced orientation in purely amorphous diblock copolymers.

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Electric field induced structural deformations in lamellar block copolymers — •X. Jiang[1], T. Thurn-Albrecht[1], T. Gutberlet[2], and M. Gupta[2] — [1]Department of Physics, Martin-Luther-University Halle-Wittenberg, 06120 Halle, Germany — [2]Laboratory for Neutron Scattering, ETHZ&PSI, CH-5232 Villigen PSI, Switzerland

Phase separation in block copolymers is restricted to molecular length scales, as a result self-assembled nanoscopic structures of different symmetries are formed in these materials. For thin films electric fields turned out to be an especially effective tool to control the orientation and order of these materials, though the details of the alignment process are not yet completely understood.

Using the time-of-flight (TOF) mode on the AMOR neutron reflectometer at the Paul-Scherrer-Institute, we studied the influence of an electric field on poly(styrene-block-methylmethacrylate) with a lamellar microstructure misaligned with respect to the electric field, in the specular and off-specular scattering regions. Even in films aligned parallel to the substrate thermally excited structural fluctuations - undulations with small amplitudes exist. A weak electric field leads to a more perfect alignment of the lamellae perpendicular to the field, which we understand as a consequence of defect suppression by the field. In addition the amplitude of the above mentioned undulations is increased by effect of the field. As expected this effect can eventually lead to a disruption and a partial alignment of the lamellar structure.

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Correlated defect dynamics in block copolymer melts — •Larissa Tsarkova, Armin Knoll, and Robert Magerle — Physikalische Chemie II, Universität Bayreuth

Block copolymers are fluid materials which self assemble into a variety of highly ordered and complex structures. Very little is known about mechanisms by which order evolves in morphologies on a nanometer scale. With scanning force microscopy we image in-situ the microdomain dynamics in a thin film of polystyrene-*block*-polybutadiene diblock copolymer while annealing above the glass transition of polystyrene. With unprecedented time resolution we follow the detailed dynamics of characteristic defects with life-time ranging from seconds to hours and lengthscale of correlated motion about several domain spacings (100 nm). Topological constrains favore various annihilation mechanisms: through local transient phases such as spherical domains, lamella, disordered state, or elastic deformations of the microdomains. Comparison of the typical time between the repetitive defect states with characteristic diffusion coefficients suggests that the motion proceeds via correlated movement of clusters of chains.

CPP 5.30 Fr 17:15 Poster TU D

Dynamics of Dense Spatial Networks in Structured Fluids: Data reduction and Visualization — •R. Magerle, H. Schoberth, and S. Scherdel — Physikalische Chemie II, Universität Bayreuth

Block copolymers and surfactant mesophases have spatially complex structures. The density distribution of components is usually displayed as an isodensity surface. However, the resulting networks are often very dense and obstruct the view into the volume of the data set. Therefore, the structure and dynamics of defects and grain boundaries is very difficult to follow. We reduce the data to their minimal features: connections are represented as thin smooth lines and branching points as small spheres of different color. The network dynamics is rendered with a tool for protein visualization. Thereby large data streams are efficiently reduced and can be grasped within seconds. As an example we present the dynamics of a transient defect in a thin film of block copolymer. The microdomain structure resembles the gyroid-to-cylinder transition investigated recently by M. Matsen [PRL 80, 4470 (1998)]. Our computer simulation based on dynamical density functional theory predicts the same structure and orientation of the defect, however, a different dynamics where one connection forms after the other.

CPP 5.31 Fr 17:15 Poster TU D

Phase Transitions of Block Copolymers under the Influence of External Noise — •Martin Kreis, Nicolaus Rehse und Robert Magerle — Physikalische Chemie II, Universität Bayreuth, D-95440 Bayreuth, Germany

Block copolymers tend to microphase separate and to form a rich variety of ordered structures on the mesoscale in thermodynamic equilibrium. We investigate thin films of polystyrene-*block*-polybutadiene with film thicknesses (< 100 nm) and lengths of the involved polymer blocks being convenient control parameters. As the films are swollen in a non selective solvent vapor they form a highly concentrated, viscous solution. Our interest is the dynamics of phase transitions between the different morphologies under the influence of external noise which is realized by either fluctuating the vapor pressure or the temperature. These transitions are followed in situ by tapping mode scanning force microscopy.

CPP 5.32 Fr 17:15 Poster TU D

Scanning Probe Microscopy of Block Copolymer Phase Separation: Force Modulation vs. Tapping Mode — •Daniel Podzimek, Hendrik Hähl, Oliver Bäumchen, Armin Nagel, and Karin Jacobs — Saarland University, POB 151 150, D-66041 Saarbrücken

Microdomain ordering due to the phase separation of incompatible blocks of polymers in thin films can be studied by scanning probe microscopy (SPM). Typically, the different blocks are characterized by different elastic properties which can be revealed by SPM. Commonly, the SPM is used in 'intermittent contact mode'. Here, the surface topography is scanned with an oscillating probe that 'taps' the surface. The oscillation amplitude is used as control signal. This technique is used for different applications, especially for imaging delicate and fragile samples like weakly adsorbed DNA molecules, colloidal particles or surfaces of polymer materials. Another possibility is to use the SPM in 'force modulation mode'. There, the probe exercises a small oscillation in the vertical direction with a frequency that is much higher than the scanning frequency and much lower than the cantilever resonance frequency, while staying in contact with the surface. The amplitude of the cantilever oscillation varies according to the elastic and friction properties of the sample. In this study we evaluate the two modes on thin films of a linear PS/PEP block copolymer.