CPP 34: POSTERS Polymerphysics

Time: Thursday 17:00–19:30 Location: Poster A

CPP 34.1 Thu 17:00 Poster A

About the Generalized Cauchy Relation in Non-Equilibrium Amorphous Materials — •Martine Philipp[1], Christelle Vergnat[1], Ulrich Müller[1], Ravi Bactavatchalou[1], Wulff Possart[2], Roland Sanctuary[1], Jörg Baller[1], Bartosz Zielinski[1], Patrick Alnot[3], and Jan Krüger[1] — [1]LPM, Université du Luxembourg, L-1115 Luxembourg — [2]Universität des Saarlandes, Saarbrücken, Germany — [3]Université Nancy, France

From solid state physics it is known that Cauchy relations (CR) increase the symmetry of the elastic tensor compared to the actual point symmetry. These CR hold true only under severe conditions concerning local symmetry and harmonicity of the elastic interaction potential. Since amorphous materials show no translational invariance the existence of CRs is not expected for these materials. Nevertheless, the authors have found for amorphous solids and high frequency clamped liquids a generalized CR (gCR) under the form of a linear transformation c11=3c44+A, with A being a constant. Once A is known, one of the two elastic constants can be predicted by knowing the other. This surprising result means that for amorphous materials the independency of the two elastic constants is strongly reduced. In the current presentation we discuss to which extent thermodynamic non-equilibrium violates the gCR. For that purpose the interdependency of c11 and c44 of reactive polymers is studied in the course of the curing process by Brillouin spectroscopy. Special attention is paid to accompanying transition phenomena like gelation and chemically induced freezing. An attempt is made to interpret the parameter A.

CPP 34.2 Thu 17:00 Poster A

cellular polyethylene-naphthalate piezo- and ferroelectrets: foaming in supercritical carbon dioxide, structure improvement through inflation and stretching — •peng fang[1], werner wirges[1], reimund gerhard[1], and larissa zirkel[2] — [1]Applied Condensed-Matter Physics, Institute of Physics, University of Potsdam, Am Neuen Palais 10, 14469 Potsdam, Germany — [2]Institute of Polymer Materials, Friedrich-Alexander University Erlangen-Nürnberg, Martensstrasse 7, 91058 Erlangen, Germany

Cellular polymer films can be used as ferroelectrets in many transducer applications. Here, we propose a preparation process for cellular polyethylene-naphthalate (PEN) films with the following steps: (1) Foaming by means of supercritical carbon dioxide (CO2), (2) controlled inflation through gas diffusion and expansion, and (3) biaxial stretching. We demonstrate and describe the cellular structure that is formed under suitable processing conditions. For the foaming process, a PEN film is saturated with supercritical CO2 at room temperature for a few hours, at a pressure as high as 100 bar, where the temperature is very critical for controlling the sample density. Additional inflation can improve the cellular geometry. Stretching may be employed in order to achieve a cellular structure with lens-like voids. Piezoelectric coefficients of up to 140 pC/N demonstrate the suitability of such cellular PEN films for transducer applications. However, high electromechanical responses are found only on samples within the proper density range and with optimal cellular structures. Their piezoelectricity is partially stable at elevated temperatures as high as 100°C.

CPP 34.3 Thu 17:00 Poster A

Röntgenabsorptionsmessungen an freien Aminosäure-Nanopartikeln — •René Lewinski, Christina Graf, Burkhard Langer, Bernhard Wassermann, Harald Bresch, Roman Flesch und Eckart Rühl — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

Die Immobilisation von Aminosäuren auf Nanopartikeln ist ein Modell für die Wechselwirkung von Biomolekülen mit Oberflächen. Zum Verständnis der Bindungsverhältnisse in solchen Systemen wurden Nanopartikel aus reinen Aminosäuren sowie nur an der Oberfläche mit Aminosäuren funktionalisierte Nanopartikel in die Gasphase gebracht und mit Innerschalenanregung studiert. Diese wurden in einem Nanopartikelstrahl erzeugt und anschließend mittels eines aerodynamischen Linsensystems ins Hochvakuum überführt. So ist es möglich, auch geringe Substanzmengen elementspezifisch zu charakterisieren, wobei Strahlenschäden sowie die Wechselwirkung mit einem anderen Substrat ausgeschlossen werden. Zunächst erfolgte eine Untersuchung der elektronischen Struktur der reinen Aminosäuren Cystein und Methionin. Dabei wurde auch studiert, wie sich der pH-Wert bei der Partikelbildung auf die elektronische Struktur von Nanopartikeln aus aggregierten Aminosäuren auswirkt. Schließlich wurden Silicananopartikel charakterisiert, deren Oberfläche eine Submonolage Methionin gebunden ist. Die Resultate zeigen, dass die genutzte Methode zur Charakterisierung der elektronischen Struktur von kleinen Mengen an empfindlichen Biomolekülen auf Nanopartikeln gut geeignet ist.

CPP 34.4 Thu 17:00 Poster A

Structure formation upon sputtering of iron in diblock copolymer film with and without maghemite nanoparticles - an in-situ GISAXS study — •Mottakin M. Abul Kashem[1], Gunar Kaune[1], Alexander Diethert[1], Weinan Wang[1], Kai Schlage[2], Sebastian Couet[2], Ralf Röhlsberger[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department LS E13, James-Franck-Str. 1, 85747 Garching, (Germany) — [2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg (Germany)

Sputtering technique can be used to incorporate metal particle fillers into a self-assembled block copolymer film to get a nanocomposite. We have investigated the structures formed during sputtering of iron on the diblock copolymer films with and without iron oxide nanoparticles. We used cylindrical structure forming diblock copolymer polystyrene-block-poly-methyl methacrylate and maghemite nanoparticles to produce the films. The metal iron was sputtered on to the surface of nanostructured film and the structure formation was recorded and investigated with in-situ grazing incident small angle X-ray scattering (GISAXS) technique. The surface topography of the composite films before and after sputtering is investigated by atomic force microscopy (AFM). The presence of nanoparticles in the film act as a nucleation site which leads to a different type and size of structures with compared to the film without nanoparticles upon sputtering of iron. Funding by the CompInt network is acknowledged.

CPP 34.5 Thu 17:00 Poster A

Poly(N-Isopropylacrylamide) as thermo responsive coating on Microcantilever Sensors — •Sebastian K. Nett[1,2], Calvin Bradley[1], Mine Memesa[1], Yajun Cheng[1], Sebastian Lenz[1], Rüdiger Berger[1], and Jochen S. Gutmann[1,2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz — [2]Institute for Physical Chemistry, Johannes Gutenberg University, Jakob-Welder-Weg 10, D-55099 Mainz

Micro fabricated cantilevers proofed to be a versatile system to be used as sensors. Any stress applied to the cantilever is very precisely detectable. Our system is consisting of an array of eight microcantilever (MCS) with a width of 90 μm, a length from 500 to 1000 μm and a thickness from 1 to 10 μm. Combined with a functional layer it is possible to build a very specific sensing system. Poly(N-Isopropylacrylamide) (PNIPAM) is known to be a polymer which exhibits a coil to globule transition in water at around 32°C [1]. PNIPAM is grafted from the silicon surface of the MCS by atom transfer polymerization (ATRP). The surface layer was analyzed on the single cantilever by μ-focus GISAXS [2] and imaging ellipsometry to determine the layer thickness. We monitored the transition by heating the coated cantilever in water. The bending was detected by the so called deflection method. At the transition temperature a change in bending is clearly observed. The reasons for the bending are discussed as a function of grafting density and layer thickness. [1] Heskins, M., et. al., J. Macromol. Sci. Chem. A2 1968, 1441. [2] Wolkenhauer, M., et. al., Applied Physics Letters 2006, 89.

CPP 34.6 Thu 17:00 Poster A

About the importance of thermodynamic properties for the understanding of nanoparticle-matrix interaction — •Bartosz Zielinski[1], Jörg Baller[1], Martine Philipp[1], Ravi Bactavatchalou[1], Ulrich Müller[1], Jan Krüger[1], Wulff Possart[2], and Roland Sanctuary[1] — [1]LPM, University of Luxembourg, Luxembourg — [2]Universität des Saarlandes, Saarbrücken, Germany

Despite the tremendous importance of thermoset-based nanocomposites there is still a huge lack of understanding concerning the relation between the desired phenomenological properties and the implementation of unexpected structures due to the nanoparticles. We will show, that from the viewpoint of phenomenology investigations of static and dynamic thermodynamic properties are amongst the most promising. Combining selected scenarios of DSC and TMDSC provide a new view into the interaction mechanisms between nanoparticles and matrix. These results give access to the interpretation of the active role of the nanoparticles on network formation. As a model system we have chosen an epoxy thermoset filled with alumina nanoparticles.

CPP 34.7 Thu 17:00 Poster A

Self-assembly of liquid crystals induced by chemically patterned substrates — •Manuel Greschek and Martin Schoen — Stranski-Laboratorium für Physikalische und Theoretische Chemie Technische Universität Berlin, Strasse des 17.Juni 135, D-10623 Berlin

We present Monte Carlo simulations for ellipsoids of revolution interacting with chemically patterned planar walls. The simulations are performed in the grand-canonical and in the isostress-isostrain ensemble. In simulations with constant stress the volume of the simulation box may change in the direction of the wall normal. Two anchoring mechanisms are investigated, namely, homeotropic alignment (symmetry axis of the particle parallel to the wall normal) across a strip of width d_{wet}, homogeneous planar alignment (symmetry axis is perpendicular to wall normal) outside this strip. The fluid particles interact via a shifted Lennard-Jones (12,6) potential modified to account for the anisotropy of the interaction. The fluid-wall interaction is modelled via a Lennard-Jones (10,4) potential and modified to account for the preferred orientation of the fluid particles. Due to larger geometric incompability stratification is more diffuse than in "simple"fluids . Molecular frustration at the junction between homeotropic and planar orienting portions of the walls decreases with increasing film thickness.

CPP 34.8 Thu 17:00 Poster A

Effective single-particle dynamics according to the Hori-type Langevin equation — •Jörg R. Silbermann[1], Sabine H. L. Klapp[1,2], and Martin Schoen[1] — [1]Stranski-Lab für Physikalische und Theoretische Chemie, Technische Universität Berlin, Strasse des 17. Juni 124, 10623 Berlin — [2]Institut für Theoretische Physik, Technische Universität Berlin, Strasse des 17. Juni 124, 10623 Berlin

We consider the dynamics of a single tagged particle of mass M in a 2D Lennard-Jones (LJ) system. Employing the Mori-Zwanzig projector operator formalism, it is possible to derive an effective equation of motion of the form of a generalized Langevin equation (GLE). The "random force" $F_0^r(t)$ appearing in the GLE is in general unknown. For a harmonic solid, however, one can derive [1] a GLE where $F_0^r(t)$ coincides with the total force $F_0^*(t)$ acting on the tagged particle in a "reference system", where the mass is changed from M to an arbitrary mass m^*. We study to what extent this GLE is still able to capture the dynamics of the tagged particle under conditions where the harmonic approximation is no longer justified. To this end we compute typical time-autocorrelation functions for the tagged particle in molecular dynamics simulations for the full LJ system and compare these with the ones obtained by solving the GLE. We find excellent agreement at low temperatures and surprisingly good reproduction of the dynamics even in the high-temperature liquid phase.

[1] K. Wada, J. Hori, Prog. Theor. Phys. **49**, 129 (1973).

CPP 34.9 Thu 17:00 Poster A

Dipolar ordering between three and two dimensions — •R. Andreea Trasca[1] and Sabine H.L. Klapp[1,2] — [1]Stranski-Laboratorium für Physicalische und Theoretische Chemie, Sekretariat C7,Technische Universität Berlin,Strasse des 17. Juni 115, D-10623 Berlin, Germany — [2]Institut für Theoretische Physik, Sekretariat PN 7-1, Facultät II für Mathematik und Naturwissenschaften, Technische Uniersität Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

We perform Monte Carlo simulations to investigate the orientational and translational ordering behavior of dipolar soft-sphere films confined between planar walls with gaps between 5 and 1.5 σ [1]. At 5 σ the dipolar film exhibits a spontaneous ferromagnetic transition similar to ones previously found at larger gaps and in bulk [2]. As the gap is decreased the ferromagnetic order vanishes, but a high degree of dipolar allignment is preserved, as antiferromagnetic stripes.

Besides the orientational ordering, the dipolar film forms layers due to soft-sphere interactions. The translational order in the plane of the layers is investigated using pair correlation functions and bond angle order parameters. As a reference we also compute the translational order of confined soft-sphere films. At very high densities, starting from the equilibrated soft-sphere configuration and random dipoles,a nontrivial change of the translational as well as the orientational structure of the dipolar soft-sphere film is observed.

1. R.A. Andreea and S.H.L. Klapp, in preparation.
2. S.H.L.Klapp and M.Schoen, J.Chem.Phys. 117, 8050 (2002).

CPP 34.10 Thu 17:00 Poster A

Surface-pattern recognition by molecular fluids — •Timo Poppmann and Martin Schoen — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Germany

We investigate the phase behavior of molecular, rodlike fluids confined between nonplanar substrates by means of canonical ensemble Monte Carlo(CEMC) simulations. Substrates are infinitely long in the y-direction and consist of a periodic sequence of wedge-shaped furrows of depth D and periodicity s_x in the x-direction. Moreover, the substrates stay in register in the x-direction. The interaction potentials are of the Lennard-Jones type with an anchoring orientation function g($\hat{u}$). We find a clear correlation between the preferred orientation of molecules and the fluid density in the vicinity of the substrates.

CPP 34.11 Thu 17:00 Poster A

Multimode analysis of Ni-, Pd-, and Pt- phthalocyanines — •Davoud Pouladsaz, Thiruvancheril Gopakumar, Michael Hietschold, and Michael Schreiber — Institut für Physik, Technische Universität Chemnitz

We investigate the photoelectron spectra of the first ionization of Ni-, Pd-, and Pt- phthalocyanines by a multimode analysis as the computation of vibronic coupling constants and reorganization energies with density functional theory (DFT).

CPP 34.12 Thu 17:00 Poster A

Structure and thermodynamics of concentrated electrolyte solutions — •Immanuel Kalcher and Joachim Dzubiella — Physics Department, TU Munich

Concentrated electrolytes are a substantial component of many molecular systems, e.g. in cell biology, nanofluidics, or clays. The prediction of their equilibrium structure and thermodynamics in bulk and confinement remains a difficult task. We address this challenge by performing extensive explicit-water molecular dynamics (MD) computer simulations of electrolytes for a wide range of salt species and concentrations (<6M). The bulk ion-ion radial distribution functions (rdfs) are calculated and then used as input in statistical mechanics approaches to predict macroscopic thermodynamics and the inhomogeneous electrolyte structure in confinement. Here we utilize the interesting observation that the water-induced short-ranged structure of the bulk electrolyte is only weakly dependent on salt concentration. By applying a simple Debye-Hueckel approach with a concentration dependent permittivity we show that the different radial distribution functions can be mapped onto each other by separating the short and long range contributions. This mapping enables us to reproduce the experimental osmotic pressures of electrolyte solutions fairly well over a range of 0-3 mol with the knowledge of only two accurate bulk rdfs. Furthermore, strong structural inhomogeneities are observed in MD simulations of concentrated electrolytes in nanometer-sized confinement and are compared to solutions of Poisson-Boltzmann based approaches.

CPP 34.13 Thu 17:00 Poster A

Influence of the nanoscale lamellar orientation of UHMW-PE surfaces on the protein adsorption — •Thomas Keller, Matthias Grosch, Erik Vater, David Trimbach, and Klaus D. Jandt — Institut für Materialwissenschaft und Werkstofftechnologie (IMT), Friedrich-Schiller-Universtität Jena, Löbdergraben 32, 07743 Jena

The here presented study shows that for thin-melt drawn films of ultra-high molecular weight polyethylene (UHMW-PE) - an implant material already in use - the lamellar crystal arrangement on the surface can be influenced on the nano-scale by processing conditions. These lamellae protrude from the film surface and therefore, such highly oriented UHMW-PE films open up the possibility to investigate the interaction of nano-topographic features with proteins and cells. The in arthroplasty most relevant protein human serum albumin (HSA) was systematically adsorbed on these UHMW-PE surfaces and analyzed by means of atomic force microscopy (AFM). Solutions of different HSA concentrations in PBS buffer were brought onto the highly ordered UHMW-PE surfaces and left for adsorption for different periods of time. By varying the concentration and time for protein adsorption, a partial to full surface coverage was achieved. On the partially HSA-covered UHMW-PE surfaces a preferential alignment of the proteins with the lamellar thickness parallel to the drawing direction was observed. Thus, new insight into the interaction of proteins with nanoscale topographic features of UHMW-PE surfaces was gained.

CPP 34.14 Thu 17:00 Poster A

Direct observation of phonon decay in two-dimensional colloidal crystals — •Julian Dietrich[1], Jörg Baumgartl[1], Hans-Hennig von Grünberg[2], and Clemens Bechinger[1] — [1]2. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Institut für Chemie, Karl-Franzens-Universität, 8010 Graz, Austria

Lately there is growing interest in the band structures of so called phononic crystals which exhibit a phononic band gap. In a recent study it has been shown that such phononic band gaps can also be induced in colloidal crystals through anisotropic interactions including substrate-particle and particle pair interactions. In our experiment we investigate a new approach to determine the band structure of such a two-dimensional colloidal crystal directly from the phonon dynamics. Since colloidal suspensions are overdamped systems the phonons do not propagate but decay exponentially with a characteristic decay time inversely connected to the phonon band structure. We directly measure these decay times using video microscopy. Moreover, we apply a commensurate hexagonal substrate created with three interfering laser beams in order to tune the decay times. Finally, we investigate the behaviour of the decay times for vanishing substrate strengths; preliminary results indicate that hydrodynamical effects become important in the centre of the first Brillouin zone, i.e. for long wavelength phonons.

CPP 34.15 Thu 17:00 Poster A

Light-Induced Surface Relief Gratings on Novel Low-Molecular-Weight Organic Glasses Containing Azobenzene Side Groups — •Hubert Audorff[1], Lothar Kador[1], Roland Walker[2], and Hans-Werner Schmidt[2] — [1]Institute of Physics and BIMF, University of Bayreuth, 95440 Bayreuth — [2]Macromolecular Chemistry I and BIMF, University of Bayreuth, 95440 Bayreuth

A number of novel low-molecular-weight glass formers with azobenzene moieties has been synthesized to examine the formation of surface relief gratings (SRGs). In addition to birefringent volume gratings, SRGs with heights up to 650 nm were formed in holographic experiments. The amplitudes of the latter were calculated from the diffraction efficiencies and independently measured by atomic-force microscopy. The temporal evolution of the diffraction efficiencies of both types of gratings was monitored. The gradient force model is capable of explaining all the experimental results. The differences between the gratings generated with different writing polarizations can be ascribed to the varying strengths of the gradient force. The influence of the molecular end groups on the SRG formation was investigated. Temperature-dependent measurements allow the determination of the glass transition temperature. At elevated temperatures, the SRG formation rate drops due to increased fluidity of the material.

CPP 34.16 Thu 17:00 Poster A

Temperature dependent optical spectroscopy of rubrene single crystals — •Olga Krylova[1], Jens Pflaum[2], Rainer Stöhr[2], Linus Gisslen[3], Reinhard Scholz[3], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Bonn — [2]3. Physikalisches Institut, Universität Stuttgart — [3]Walter Schottky Institut, Technische Universität München

High quality rubrene crystals were grown by sublimation under streaming hydrogen. Polarized and angle-resolved fluorescence and absorption spectra were measured as a function of temperature. The fluorescence spectrum shows a strong reversible variation with temperature. The spectral changes are accompanied by a very strong (1000 fold) increase of the luminescence intensity at low T. At room temperature, the luminescence can be understood by the formation of H-aggregates of the transition dipoles due to efficient coupling in the (b,c)-crystal plane. This leads to emission from the zone boundary and hence causes a low luminescence yield and a large Stokes shift. At low temperatures, the luminescence spectrum is more reminiscent to that of a J-aggregate. This would imply that at low T, there exists a minimum of the exciton dispersion at the center of the Brillouin zone, which allows luminescent decay with high efficiency. We plan time-dependent PL measurements, which allow us assign temperature-dependent decay rates of the various PL bands, allowing estimates of the respective radiative lifetimes and the activation energies of non-radiative quenching mechanisms. Supported by DFG through the research unit 557.

CPP 34.17 Thu 17:00 Poster A

Light-induced modifications of the molecular switch 3-(4-(4-Hexylphenylazo)phenoxy)propan-1-thiol adsorbed on Au(111) studied by two photon photoemission — •Nils Heinemann[1], Oleksiy Andreyev[1], Ulrich Jung[1], Claudia Bornholdt[2], Olaf Magnussen[1], Rainer Herges[2], and Michael Bauer[1] — [1]Institut für Experimentelle und Angewandte Physik, Uni Kiel — [2]Otto-Diehls Institut für Organische Chemie, Uni Kiel

Molecular switches and their intriguing properties attract much interest in the field of molecular electronics. Whereas the reversible switching of molecules has been well studied in gases and liquids, the successful realization and sensing of molecular switching at surfaces still remains a challenging task. Quite recently, Hagen et al. reported on the observation of a photoinduced reversible switching of tetra-tert-butyl-azobenzene molecules adsorbed on a Au(111) surface by means of the two photon photoemission technique (2PPE) [1].

In this contribution we will present 2PPE results of the molecular switch 3-(4-(4-Hexylphenylazo)phenoxy)propan-1-thiol adsorbed on Au(111). A tuneable 80 MHz fs-laser system is employed to study changes in the electronic structure of the adsorbed molecule induced by laser illumination at 365 nm and 435 nm. We observe a distinct and wavelength characteristic impact on the 2PPE spectra, which also depends critically on the applied light intensity. The results will be discussed particularly in the context of a switching of the adsorbed molecule.

[1] S. Hagen et al., Chem. Phys. Lett. 444 (2007) 85-90.

CPP 34.18 Thu 17:00 Poster A

MD Simulations of Sheared Polymer Brushes with Explicit Solvent — •Andre Galuschko, Torsten Kreer, Joachim Wittmer, and Joerg Baschnagel — Institut Charles Sadron, 6 rue Boussingault, F-67083 Strasbourg Cedex, France

Polymer brushes play an important role as lubricants in many technical applications, e.g. in hard disk drives or artificial joints [1]. They are furthermore believed to be crucial for minimizing friction between synovial joints [2], such as human knees or hips.

Using Molecular Dynamics simulations of a standard coarse grained model we study the lubrication properties of short chain polymer brushes. We extend further approaches (see, e.g. Refs.[3-5]), which have been performed without explicit solvent, to new simulations, where we now account for hydrodynamic interactions via including solvent molecules. We investigate the static properties of isolated and compressed brushes, and study the response of these systems to stationary and non-stationary external shear. This is done under variation of the molecular parameters, i.e. grafting density and chain length. By comparing to previous simulation results of the same model without explicit solvent, we aim at understanding the role of hydrodynamic interactions in polymer brush lubrication.

[1] T. Moro et al., Nat. Mater. 3, 829 (2004).
[2] J. Klein, Proc. IMechE J 220, 691 (2006).
[3] G.S. Grest, Phys. Rev. Lett. 76, 4979 (1996).
[4] P.S. Doyle et al., Phys. Rev. Lett. 78, 1182 (1997).
[5] T. Kreer et al., Langmuir 17, 7804 (2001).

CPP 34.19 Thu 17:00 Poster A

Force Studies on Responsive Polymeric Brush Surfaces — •Mukesh Kumar Vyas, Konrad Schneider, Bhanu Nandan, and Manfred Stamm — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden, Germany

Surface forces such as adhesion and friction play important roles in the manipulation, assembly, and operation of micro- and nanoscale devices. We perform atomic force microscope (AFM) based force studies on polystyrene * poly(2-vinylpyridine) (1:1) mixed polymer brushes and corresponding monobrushes in air. Adhesion and friction force behaviour of polymer brush surfaces in contact with inorganic and polymeric surfaces, was studied using silicon tips, silicon nitride tips, colloidal probe with silica particle and colloidal probe with polystyrene (PS) and poly(acrylic acid) brushes on surface. The effect of switching behaviour of chemical composition of binary brush surfaces (on treatment with suitable solvents) on the wettability, surface roughness, and hence on the adhesion and friction properties of the surfaces, was investigated. Surface roughness values for the entire polymer brushes samples were in the same range and had minimal influence on the trend obtained for the force values. Adhesion force values were in accordance with the wettability of the samples. Adhesion and friction values were correlated to wettability for most of the cases except for the silicon tip.

CPP 34.20 Thu 17:00 Poster A

Self-rolled Polymer Microtubes and Toroidal Microcavities — •Kamlesh Kumar, Valeriy Luchnikov, and Manfred Stamm — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden, Germany

Microtubes and microtoriods of different nature find various applications in microfluidic devices, sensors, filters, wave-guides etc. In the present work, we have investigated the fabrication of microtube and microtoroids by self-rolling of thin strained bilayer polymer films, composed of polystyrene/poly (4-vinyl pyridine) and released in controllable manner from a solid substrate. The bilayer film develops strain due to unequal swelling of polymers in selective solvents and hence the film bends and scrolls in order to minimize its free energy. These tubes and toroids were characterized in detail using optical microscopy, atomic force microscopy, and scanning electron microscopy.

Inner surfaces of tubes and toroids could be functionalized using photolithography, micro-contact printing, vacuum sputtering of metals, ion beams, plasma chemical activation etc. Photolithography, electron beam lithography and direct mechanical patterning with a sharp blade were used for the structuring of the bilayer before the rolling of tube. Looped tubes with metallized hidden walls, produced by self-rolling technique, may act as micro-resonators in the corresponding frequency range. The self-rolling approach opens new broad opportunities for mesoscale engineering of the tube-based devices, since it combines highly developed planar methods of surface modification with self-organized formation of 3D micro- and nanostructures.

CPP 34.21 Thu 17:00 Poster A

Identification of dissipative and elastic contributions in force spectroscopy curves and tapping mode AFM images for polymeric model surfaces — •Klaus Schröter, Albrecht Petzold, Thomas Henze, and Thomas Thurn-Albrecht — Institut für Physik, Universität Halle-Wittenberg

The separate identification of dissipative and elastic force contributions in Atomic Force Microscopy (AFM) is discussed. We show that within a harmonic approximation the interaction of the AFM tip with the sample surface can be described by average interaction parameters which can be extracted in a simple way from measured data. The method is applied to force spectroscopy curves on hard and soft polymeric model surfaces. The understanding of the basic effects then enables a clearer interpretation of AFM images and an identification of phases in systems with hard-soft contrast as for instance on semicrystalline polymers.

CPP 34.22 Thu 17:00 Poster A

Side chain dynamics and crystallization in nanophase-separated regio-random poly(3-alkyl thiophenes) — •Shireesh Pankaj, Elke Hempel, and Mario Beiner — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle/Saale, Germany

A series of regio-random poly(3-alkyl thiophenes-2, 5-diyl) has been investigated by differential scanning calorimetry, x-ray scattering and dynamic mechanical analysis. Samples with varying side chain lengths from $C = 4$ to $C = 12$ alkyl carbons were studied to understand details of the interplay between structure and cooperative dynamics in these nanophase-separated side chain polymers. Two glass transitions are observed for the amorphous members ($C = 4 - 8$) like in previously studied atactic poly($n-$alkyl methacrylates). In both cases, the aggregation of alkyl groups to small alkyl nanodomains with a typical dimension of about 1 nm is indicated by a prepeak in x-ray scattering data. Crystallization of alkyl groups within the alkyl nanodomains is seen for the higher thiophenes, i.e., for the decyl ($C = 10$) and dodecyl ($C = 12$) members. A special feature which is observed for the dodecyl member is that different melting peaks are seen depicting polymorphism of the crystallizable side chains. This is not observed in poly($n-$alkyl methacrylates) and poly($n-$alkyl acrylates) with similar side chain lengths. Isothermal crystallization results for these samples are presented and discussed in the light of recently developed theories of polymer crystallization.

CPP 34.23 Thu 17:00 Poster A

Optical Properties of Ink-Jet-Printable PPE-PPV/ Semiconductor Nanocrystal Hybrid Materials — •Thomas Blaudeck[1], Stephan Jahn[1], Daniel A. M. Egbe[1], Reinhard Baumann[1], and Christian von Borczyskowski[2] — [1]Institute of Print and Media Technology, TU Chemnitz, 09107 Chemnitz, Germany — [2]Optical Spectroscopy and Molecular Physics, TU Chemnitz, 09107 Chemnitz, Germany

Hybrid materials made of organic poly(p-phenylene-ethynylene-alt-poly(p-phenylene-vinylene) (PPE-PPV) and inorganic semiconductor nanocrystals are promising candidates for various applications in electronic and optoelectronic devices such as LEDs, OBDs, and transistors. Considering the high chemical structural versatility and mechanical flexibility of PPE-PPV, devices in mind have to go along with suitable low-cost production routines. In this respect, digital fabrication techniques such as ink-jet printing have gained considerable interest as they combine the demand for a high throughput with small structure sizes down to the range of several micrometers. Whilst the suitability of PPE-PPV for printing was recently proven [1], additives and impurities were found to considerably affect the optical, functional, and rheological properties of the printing formulation. Apart from some empirical data, their particular role is still poorly understood. In this study, we focus on the influence of semiconductor nanocrystals on the optical properties of a series of ink-jet printable PPE-PPV formulations and their precursors.

[1] E. Tekin et al., Journal of Materials Chemistry 16, 4294 (2006).

CPP 34.24 Thu 17:00 Poster A

Static and dynamic properties of tethered chains in different surface regimes. Monte Carlo studies. — •Radu Descas[1], Jens-Uwe Sommer[2], and Alexander Blumen[1] — [1]Theoretische Polymerphysik, Universität Freiburg, Hermann-Herder-Strasse 3, D-79104 Freiburg — [2]Leibniz-Institut für Polymerforschung Dresden, Hohe Strasse 6, D-01069 Dresden

Using MC simulations combined with scaling arguments we study the adsorption of tethered polymer chains at flat surfaces. The interplays between the grafting density σ, the excluded volume, and the strength of adsorption κ lead to different surface regimes. We suggest a $\sigma - \kappa$ phase diagram and focus on the semidilute surface regime and on the oversaturated brush regime. In these regimes we study both the static [1] and the dynamic [2] properties of the chains. Using scaling arguments and computer simulations we analyse the average extension of single chains both parallel and perpendicular to the surface. Especially for the parallel component our simulation results agree well with the scaling predictions. In the semidilute regime the dynamics is well described by a model in which the chains form adsorption blobs. In the oversaturated brush regime the system can be visualized as a brush-like state formed on top of a saturated adsorption layer. Our simulations show that in this regime the dynamics is controlled by three-dimensional blobs.

[1] R. Descas, J.-U Sommer, and A. Blumen, J. Chem. Phys. **125**, 214702 (2006).

[2] R. Descas, J.-U Sommer, and A. Blumen, in preparation.

CPP 34.25 Thu 17:00 Poster A

Hyperquenching in linear polyethylene and ultrafast calorimetry at heating and cooling rates up to 2 millions K/s — •Alexander Minakov[1,2] and Christoph Schick[1] — [1]University of Rostock, Institute of Physics, Universitätsplatz 3, 18051 Rostock, Germany — [2]A.M. Prokhorov General Physics Institute, Vavilov 38, 119991 Moscow, Russia

Ultrafast nanocalorimetry was applied for hyperquenching in ultra high molecular weight linear polyethylene (UHMWPE). We determine the quenching rate required to obtain amorphous polyethylene from the melt. UHMWPE can be strongly supercooled at high cooling rates. The peak in heat capacity cp(T) corresponding to crystallization shifts to lower temperatures with increasing cooling rate in the range 10ˆ3 - 10ˆ5 K/s. This shift attains saturation at the rate 10ˆ5 K/s. At subsequent increasing cooling rate the peak in cp(T) decreases. Crystallization can not be accomplished for 10 μs. Totally amorphous PE sample at cooling and subsequent heating rate ca. 2*10ˆ6 K/s was obtained for samples of 0.1 ng and 0.06 ng (the samples thickness was ca. 0.1 μ). Considerable superheating of the melting in UHMWPE was observed. We have performed superheating measurements for 2.5 ng and 0.06 ng samples melt-crystallized for 1 min at 96°C and 106°C in the range 2*10ˆ3 - 2*10ˆ6 K/s of the heating rate. The rate dependence of superheating increment is described by the power law with exponent 0.212.

CPP 34.26 Thu 17:00 Poster A

Thermo-optical and thermo-mechanical properties of smec-

tic liquid-crystal — •Jörg Petzold[1], Tilo Finger[1], Ralf Stannarius[1], Patrick Beyer[2], and Rudolf Zentel[2] — [1]Otto-von-Guericke Universität Magdeburg — [2]Johannes Gutenberg-Universität Mainz

Incorporation of liquid-crystal mesogens in polymer backbones and subsequent cross-linking leads to the preparation of main chain liquid crystalline elastomers (LCE). Such compounds show unique effects because of the interaction of mesogenic and elastomer properties.

We report mechanical, x-ray and optical measurements of freely suspended filaments of such LCE. Among the interesting effects are the reversible elongation of the filaments along the smectic-isotrop phase transition (thermoelasticity) and a strain induced birefringence due to the coupling of mesogen orientation and applied stress. Elastic and optical parameters are derived from the stress-strain characteristics.

For additional information: "Monodomain Liquid Crystal Main Chain Elastomers by Photocrosslinking" by Patrick Beyer, Eugene M. Terentjev, Rudolf Zentel

CPP 34.27 Thu 17:00 Poster A

Observation and visualization of block copolymer microdomain dynamics — •Eike-Christian Spitzner, Christian Riesch, Christian Dietz, Nicolaus Rehse, and Robert Magerle — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

We investigate the microdomain dynamics in thin films of polystyrene-*block*-polybutadiene copolymers which form hexagonally ordered polystyrene cylinders in bulk. The films are swollen in chloroform vapour and observed in situ with tapping mode scanning probe microscopy. A temporal resolution of 15 s per frame is achieved. Image sequences show the dynamics of structural phase transitions and individual point defects. Phenomena such as defect annihilation, fluctuations of cylinder thickness and meandering of cylinders are of particular interest. From local Fourier transformations we obtain colour-coded maps of the cylinder orientation. With Nanotomography, consisting of consecutive steps of etching and imaging, we acquire volume images of microdomain structures.

CPP 34.28 Thu 17:00 Poster A

Modelling charge transport in polypyrrole — •Victor Rühle[1], James Kirkpatrick[1,2], Kurt Kremer[1], and Denis Andrienko[1] — [1]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — [2]Centre for Electronic Materials and Devices, Department of Physics, Imperial College London, London SW7 2BW, UK

Polypyrrole is one of the most stable and easy to synthesize conductive polymers. The charge transport in its reduced and oxidized states is however not fully understood. The main problem is to link the morphology to the conducting properties, since different time and length scales are involved: the individual electron hops occur on a quantum scale and hence strongly depend on the local structure. However, the entire path which charges follow is strongly affected by the large scale morphology.

In this work, an atomistic model to generate morphologies of PPy is first developed. Ab-initio methods are used to derive an atomistic force field for the neutral as well as the oxidized polymer. To be able to generate large scale morphologies, coarse graining of this atomistic model is then performed. Finally, both models are applied to small samples of PPy and the physical properties are compared. Once whole morphologies are generated, the charge mobility is calculated combining Marcus theory with a Master equation approach.

CPP 34.29 Thu 17:00 Poster A

Molecular dynamics of ultrathin supported polysulfone films studied by dielectric spectroscopy — Diana Labahn and •Andreas Schönhals — Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin

Broadband dielectric spectroscopy (10 mHz to 10 MHz) was employed to study the glassy dynamics of ultra thin supported polysulfone layers. The ultra thin films were prepared between two aluminum electrodes. Glass slides, cleaned in an ultrasound alkaline bath, rinsed in pure chloroform, and dried under nitrogen flow, were used as supporting substrates. Thin polymer films were spin-coated from a chloroform solution at 3000 rpm. The film thickness from microns down to below 10 nm was adjusted by changing the concentration of the polymer in solution. After spin-coating, the samples were annealed at a temperature well above the bulk glass transition. As a main result, for carefully annealed samples no change of the glass transition temperature with the decreasing film thickness is observed in contradiction to literature results. A more detailed analysis using a derivative technique shows that the Vogel temperature increases und the fragility parameter decreases with decreasing film thickness.

CPP 34.30 Thu 17:00 Poster A

Dielectric and Gas transport Properties of Polymeric Nanocomposites based on Polyhedral Oligomeric Silsesquioxanes — Ning Hao, Martin Böhning, and •Andreas Schönhals — Federal Institute for Materials Research and Testing (BAM), 12205 Berlin, Germany

Polymer based nanocomposites continue to receive tremendous attention for different applications. They show remarkable property improvement (increased tensile properties, decreased gas permeability, decreased solvent uptake, increased thermal stability and flame retardance) when compared to conventionally scaled composites. Different polymer based nanocomposites are prepared where polycarbonate and polystyrene are used as polymer matrices. As molecular nanofiller polyhedral oligomeric silsesquioxanes (POSS) with Phenethyl substituents is used. The property structure relationships of these nanocomposites are investigated by dielectric spectroscopy, gas transport measurements (permeation, sorption) and density measurements as well. The results are discussed with regard to the phase structure of the nanocomposites. This includes the construction of phase diagrams. For the first time a correlation between dielectric and gas transport data are given.

CPP 34.31 Thu 17:00 Poster A

AFM analysis of novel Polypropylenes — •Dirk Doser[1], Stefan Fischer[1], Othmar Marti[1], Tobias Diesner[2], and Bernhard Rieger[2] — [1]Institute of Experimental Physics, University of Ulm, 89069 Ulm, Germany — [2]Wacker-Lehrstuhl für makromolekulare Stoffe, TU München

The aim of this work was to observe the complex structures of novel isotactic Polypropylenes (iPP) using tapping mode and pulsed force mode AFM. Therefore two different approaches in sample preparation were investigated. Thin film preparation on Silicon wavers with toluene solved Polypropylene served to explore the unstretched structure. The thin films were also prepared on stretchable carriers like PDMS for studying the stretched iPP. Second samples of isotactic Polypropylene microtome cuts were prepared by potassium permanganate etching. In that case some samples were stretched before preparation. The results of this measurements will be discussed.

CPP 34.32 Thu 17:00 Poster A

Micromechanics of thin films of elastomeric polypropylenes — •Mechthild Franke, Mario Zerson, Mario Jecke, Robert Magerle, and Nicolaus Rehse — Chemische Physik, TU Chemnitz, 09107 Chemnitz

Elastomeric polypropylene consists of lamellar crystals embedded in an amorphous matrix. The arrangement, distribution, and connectivity of these crystals are important factors which determine the mechanical properties of the polymer. Free standing, $\sim 1\ \mu$m thick films of different elastomeric polypropylenes are produced by dip coating the polymer solution on a NaCl crystal, floating the film onto water, and depositing it on a slotted silicon substrate. A stretching device, based on a piezoelectric drive, allows stretching the free standing film stepwise up to strains of 100%. The changes in shape, orientation, and morphology of crystalline regions are observed in situ with scanning force microscopy. Caused by the induced stress new lamellae crystallize; existing ones elongate or break into blocks. Furthermore, amorphous areas are stretched a lot more than crystalline ones. Volume images of thin films obtained with SFM based Nanotomography allow to explain some of the observed rearrangements of the microstructure.

CPP 34.33 Thu 17:00 Poster A

Nanotomography of semicrystalline polypropylene using bimodal atomic force microscopy — •Christian Dietz[1], Mario Zerson[1], Christian Riesch[1], Alexander M. Gigler[2], Robert W. Stark[2], Nicolaus Rehse[1], and Robert Magerle[1] — [1]Technische Universität Chemnitz, Reichenhainer Str. 70, 09107 Chemnitz, Germany — [2]Center for Nanoscience and Dept. Earth and Environmental Sci., Ludwig-Maximilians-Universität München, Theresienstraße 41/II, 80333 München

High resolution volume images of semicrystalline polypropylene were obtained by stepwise wet-chemical etching followed by atomic force microscopy imaging of the specimen. Compositional contrast changes from crystals that are stiff to the amorphous phase which is rather soft. The dissipated energy as function of the cantilever's oscillation amplitude allows to identify dissipation processes at the nanoscale and to distinguish crystalline from amorphous regions. To enhance resolution a bimodal atomic force microscope was used where the first two flexural eigenmodes of the cantilever are mechanically excited and the cantilever deflection signal is analyzed using two lock-in amplifiers. While the amplitude of the first mode is used as an electronic feedback signal, the amplitude and phase signal of the second eigenmode are used to distinguish compositional changes of the material. This approach allows for a higher signal to noise ratio than the phase signal of the first eigenmode and it is less influenced by the sample topography.

CPP 34.34 Thu 17:00 Poster A

Influence of substrate temperature on pulsed laser deposited PMMA films — •Britta Lösekrug, Susanne Seyffarth, Andreas Meschede, and Hans-Ulrich Krebs — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen

Poly(methyl methacrylate) (PMMA) thin films are important for applications e. g. as coating materials and in microelectronics. Here pulsed laser deposition (PLD) at a wavelength of 248 nm is used with low laser energy densities slightly above the deposition threshold of PMMA (between 80 and 160 $\mathrm{mJ\,cm^{-2}}$). Under these conditions at room temperature thin films can be produced which are completely smooth and show no droplets at all [1].

In contrast, for higher substrate temperatures above the glass transition (at 110 °C) a dewetting of PMMA thin films on Si(111) substrates occurs. Additionally, an increased hardness of these PMMA films compared to films deposited at room temperature is observed. So the properties of PMMA films change with substrate temperature during deposition. It can be shown by infrared spectroscopy (FTIR) and size exclusion chromatography (SEC) that the chemical composition of the PMMA films is still intact up to 200 °C, while the chain lengths are reduced compared to the starting material. At still higher temperatures the deposited material begins to evaporate.

[1]B. Lösekrug, A. Meschede, H.U. Krebs, Appl. Surf. Sci. **254** (2007) 1312

CPP 34.35 Thu 17:00 Poster A

Are there cross-aggregates? In-situ NMR study of the t-butyllithium initiated butadiene polymerization — •Aizhen Niu[1], J. Allgaier[1], L. Willner[1], J. Stellbrink[1], D. Richter[1], R. Hartmann[2], and L. J. Fetters[3] — [1]IFF, Forschungszentrum Jülich, D-52425 Jülich — [2]INB2, Forschungszentrum Jülich, D-52425 Jülich — [3]Cornell University, Ithaca, NY 14853, USA

The anionic polymerization kinetics and mechanism are complicated by the aggregation phenomena of organolithium compounds. In our previous work, the kinetics and aggregation states were investigated under standard polymerization conditions by the combination of in situ small angle neutron scattering (SANS) and ^{1}H NMR techniques. It is clear that the measurement of kinetic orders is not a tool that can be used to assay aggregation states as has long been assumed. We found that the existence of cross-aggregates formed from initiator and the polybutadienyllithium head groups can be the reason making the initiator become more reactive than in the pure self-aggregated state. In an attempt to understand the influence of cross-aggregattion plays in anionic polymerization, the investigation on cross-aggregation of an anionic polymerization were performed by high resolution ^{1}H NMR and Li^7 NMR. The cross-aggregation in the mixture of t-butyllithium and living chains, 3-Neopentylallyllithium and in the initiation stage of real polymerization were studied. It is clear that there are cross-aggregates and they play an important role in anionic polymerization.

CPP 34.36 Thu 17:00 Poster A

Crystallization Kinetics in Nanocomposites of Semicrystalline Polymers — •Andreas Wurm[1], Alexander Minakov[1], Dirk Lellinger[2], Tetyana Skipa[2], Ingo Alig[2], Petra Pötschke[3], and Christoph Schick[1] — [1]University of Rostock, Institute of Physics, Polymerphysics, 18051 Rostock, Germany — [2]Deutsches Kunststoff-Institut, Schloßgartenstr. 6, 64289 Darmstadt, Germany — [3]Leibniz Institute of Polymer Research, Hohe Str. 6, 01069 Dresden, Germany

In order to understand the nucleation and crystallization in CNTpolymer composites simultaneous experiments with a combination of different methods are extremely useful. As an important supplement to the classical techniques for crystallization (SAXS/WAXS or DSC), measurements of the AC conductivity and permittivity are of interest for CNT-polymer composites. These experiments allow the investigation of the changes in the conductive percolation structure by crystallization. Two effects are expected to influence conductivity and dielectric properties: (i) crystallisation near the CNT and at the CNT-polymer-CNT contacts and (ii) crystallization in the bulk. Therefore a microcalorimeter was designed, which allows to measure thermal properties like heat capacity and thermal conductivity, which can be used in a X-ray beam of a synchrotron, where simultaneously SAXS and WAXS patterns on the same sample volume can be recorded. On the other hand the microcalorimeter was extended for additional dielectric relaxation spectroscopy, again at the same time on the same sample volume.

CPP 34.37 Thu 17:00 Poster A

Crosslinkable Polymer Brushes - Synthesis and Characterization — •Sebastian G. J. Emmerling, Andreas Hanewald, and Jochen S. Gutmann — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany

Atom transfer radical polymerization (ATRP) has opened the way to macromolecular engineering of polymeric materials. In this field, molecular brushes with poly(dimethylsiloxane) (PDMS) side chains were prepared by atom transfer radical polymerization (ATRP) conditions via macromonomer method (grafting through)[1]. The properties of these molecular brushes are dominated by the PDMS side chains, giving rise to numerous applications. In most of the cases, silicones are used as coatings because of their unique surface properties. Polydimethylsiloxane (PDMS) is undoubtedly the most widely used silicone. To produce this polymer living anionic polymerization is employed. However, this method requires stringent purification and stoichiometric conditions, which is a major drawback. The wide range of applications, that illustrates the versatility of this inorganic polymer arises from its unique combination of properties such as low surface tension, low glass transition temperature, high permeability to gas, and excellent weather resistance. However, since PDMS is a fluid at room temperature, the homopolymer lacks dimensional stability. In order to produce silicone-based materials with more desirable mechanical properties, we copolymerize the macromonomer with a benzophenone crosslinker[2].

[1] Neugebauer, D., et al., Macromolecules 2005, 38, 8687.

[2] Beines, P. W., et al., Langmuir 2007, 23, 2231.

CPP 34.38 Thu 17:00 Poster A

Characterisation of empty and polymer-filled, cylindrical mesopores using small-angle X-ray scattering — •Martin Engel[1], Bernd Stühn[1], Jörg Schneider[1], Thomas Cornelius[2], and Meike Naumann[1] — [1]Technische Universität Darmstadt — [2]Gesellschaft für Schwerionenforschung mbH

With improvements in creating well-defined mesopores in the last decades their use for investigations in nanotechnology gained great attraction. They are very promising matrices offering controllable confined geometries for self-organisation processes. Before their use as matrices it is essential to characterise these systems. In current scientific literature mesoporous systems are the object of close investigations.

In our work two kinds of mesoporous systems, highly ordered 2D hexagonal cylindrical alumina on one hand and randomly distributed well defined cylindrical ion-track polycarbonate pores were investigated with small-angle X-ray scattering (SAXS) and additionally with scanning electron microscopy. The data are analysed with the help of currently accepted models modified to deal with different sample orientations. Hence important properties like opening diameter, cylinder distance, polydispersity and sample orientation, that show up in anisoptropy of the scattering image, can be characterised.

We fill this well-defined mesopores with diblock-copolymers. Static and time-resolved scattering experiments are planned to investigate structure formation in this kind of confined geometries. The influence of the confining geometry on the resulting structure and the potential of SAXS to determine these structures will be discussed.

CPP 34.39 Thu 17:00 Poster A

Immobilized fraction in crystallizable polymer nanocomposites. — •Mohamed Ismail[1], Andreas Wurm[1], Bernd Kretzschmar[2], Doris Pospiech[2], and Christoph Schick[1] — [1]University of Rostock, Institute of Physics, Universitätsplatz 3, 18051 Rostock, Germany — [2]Leibniz Institute of Polymer Research Dresden, P. O. Box 120 411, 01005 Dresden, Germany

In this contribution we demonstrate the crystallization behavior of PA

6.6 filled with different concentrations of nanoparticles (Nanofil 919) to provide a wide range of systems with different mobility. We used a temperature modulated DSC (TMDSC) technique to determine heat capacity at the glass transition of the polymer. The existence of an immobilized fraction in PA / Nanofil 919 nanocomposites was shown. We obtained crystalline fraction, C, immobilized fraction, RAF, and the mobile amorphous fraction, MA for the whole sample series. The remaining mobile amorphous fraction of the polymer part, determined from step height at glass transition *cp, seems to be independent on filler content. Also, a slight decrease in Tg was found for more than 29.2 wt.% nanoparticles. For composites with less than 29.2 wt.% nanoparticles, the Tg is independent on filler content. By annealing experiments at and below the glass transition these results were verified.

CPP 34.40 Thu 17:00 Poster A

Solidification of fast crystallizing polymers studied by differential chip nano-calorimetry — •Evgeny Zhuravlev, Saurabh Garg, Andreas Wurm, and Christoph Schick — University of Rostock, Institute of Physics, Universitätsplatz 3, 18051 Rostock, Germany

The device was developed for investigation of thermal processes during fast thermal treatments of nanosized samples. The idea of the device was taken from differential scanning calorimetry. It consists of high sensitive, low addenda heat capacity thin film sensors used as sample and reference measuring cell. Small heated area and sensitive thermopiles allow both controlled fast heating and cooling.

Electrical control circuit was slightly modified in comparison with PerkinElmer power compensated DSC. This solution gives directly changes in heat flow from/to the sample during temperature scans.

The device works in the range of scanning rates between 0.1 and 10000 K/s with nanogram samples. It positioned exactly between existing DSC and ultra-fast scanning techniques.

Scheme, main principles and working of control circuits will be presented. We show first data on In, Sn and Pb. Measurements of supercooling of Sn samples using DSC, differential power compensated fast scanning technique and ultra-fast scanning is discussed. These measurements cover 10 orders of magnitude in scanning rate. Further we present data on isothermal crystallization of iPP and nucleated iPP in a wide temperature and dynamic range.

CPP 34.41 Thu 17:00 Poster A

Theoretical study of electron transfer through polyacetylene nanowires in different contact structures — •Davoud Pouladsaz[1], Saeideh Mohammadzadeh[2], Thomas Gessner[2], Michael Schreiber[1], and Reinhard Streiter[2] — [1]Institut für Physik, Technische Universität Chemnitz — [2]Zentrum für Mikrotechnologien, Technische Universität Chemnitz

The electron transfer of polyacetylene nanowires is studied by employing the non-equilibrium Green function's technique within the density-functional-based tight-binding method. The conductance of *trans*-polyacetylene molecules, sandwiched between Au(111) surfaces in three different contact structures, is calculated for various lengths. As well, the dependence of the conductance oscillations on the length of the molecules is investigated.

CPP 34.42 Thu 17:00 Poster A

Dielectric Properties of nanocomposites based on polyethylene and layered double hydroxide — •Andreas Schönhals[1], Francis Reny Costa[2], Udo Wagenknecht[2], and Gert Heinrich[2] — [1]Federal Institute of Materials Research and Testing (BAM), Unter den Eichen 87, D-12205 Beerlin — [2]Leibniz Institute of Polymer Research, Hohe Straße 6, D-01069 Dresden

Polymer based nanocomposites continue to receive tremendous attention for different applications. They show remarkable property improvement (increased tensile properties, decreased gas permeability, decreased solvent uptake, increased thermal stability and flame retardance) when compared to conventionally scaled composites. The dielectric properties of nanocomposites based on Mg / Al layered double hydroxide (LDH) as nanofillers and polyethylene (PE) as matrix are investigated by dielectric spectroscopy (10 mHz to 10 MHz) in a large temperature range. One dielectric active relaxation processes is observed which increases in its intensity with the concentration of the incooperated LDH. It is assigned to the segmental relaxation of PE segments which fluctuate together with the surfactant. The polar surfactant used for the interaction/exfoliation enables to observe the molecular motions of the apolar PE segments located close to the LDH sheets. A quantitative analysis provides information about the amount of the interfacial region between the inorganic LDH sheets and the bulk PE matrix.

CPP 34.43 Thu 17:00 Poster A

Microstructure and anisotropic properties of Polyamide 6 films — •Astrid Naumann[1], Hussein Shanak[1], Karl-Heinz Ehses[1], Jan Lion[1], Walter Goetz[2], and Rolf Pelster[1] — [1]Universität des Saarlandes, Gebäude E2 6, 66123 Saarbrücken, Germany — [2]BASF Company, 67056 Ludwigshafen, Germany

We have studied the anisotropy and homogeneity of Polyamide films that were prepared using different stretching techniques (uniaxial, sequential biaxial, simultaneous biaxial and "double bubble"). Structural changes concerning crystallinity and orientation of crystallites are evaluated using X-ray measurements (SAXS, pole figures). We show how the microstructure correlates with the anisotropy of properties, that are sensitive to the molecular orientation (microwave permittivity and infrared absorption). We conclude with a quantitative comparison of the above industrial production techniques.

CPP 34.44 Thu 17:00 Poster A

Crystallization kinetics of monodisperse n-alkanes at high supercooling — •Sergey Adamovsky and Christoph Schick — University of Rostock, Institute of Physics, Polymer Physics Group, 18051 Rostock, Germany

Production of monodisperse n-alkanes[1] allows to study the nanoscale process of polymer crystallization by measurements on a macro scale. Because of exactly the same chain length a measurable amount of material behaves similar way. This way providing an opportunity to derive conclusions about individual crystals from the measured sample-average properties.

Mostly DSC equipment was used for calorimetric study of these materials which is limited to tens of seconds in time resolution; thus only the high temperature slow-end tail of melt crystallization was accessible.

Fast scanning calorimetric technique[2] developed in our lab was applied to study crystallization behavior of these materials. This allowed studying kinetics of crystallization from melt in a wide temperature range with crystallization halftimes from milliseconds to hours.

Results for three selected samples are presented: $C_{122}H_{146}$, $C_{162}H_{326}$ and $C_{390}H_{782}$.

[1] G. M. Brooke, S. Burnett, S. Mohammed et al., Journal of the Chemical Society-Perkin Transactions 1 (13), 1635-1645 (1996).

[2] S. Adamovsky and C. Schick, Thermochim. Acta 415, 1-7 (2004).

CPP 34.45 Thu 17:00 Poster A

Microphase separation in cross-linked polymer melts — •Abigail Klopper[1], Carsten Svaneborg[2], and Ralf Everaers[3] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [2]Department of Chemistry and Interdisciplinary Nanoscience Center (iNano), University of Aarhus, Aarhus, Denmark — [3]Université de Lyon, Laboratoire de Physique, École Normale Supérieure de Lyon, Lyon, France

Highly concentrated liquids comprising long polymeric chains can undergo a process of cross-linking, invoking the formation of a disordered solid with a frozen memory of its preparation conditions. The cross-linking creates quenched connective and topological disorder which plays a role familiar from glassy systems in breaking the translational symmetry of the initial liquid state. In mixtures of different polymer species interacting with one another, it is responsible for the inhibition of a bulk phase separation and the establishment of microphases on intermediate length scales.

We pair a replica formalism with data from large-scale molecular dynamics simulations of nearly ideal cross-linked polymer systems with purely repulsive monomer interactions. By combining simulation with theory in this way, we are able to describe neutron scattering measurements in microphase-separating systems with attractive monomer interactions, without resorting to exhaustive simulation. In doing so, we uncover system-specific effects relating to the intrinsic length scales of our networks.

CPP 34.46 Thu 17:00 Poster A

Structure and dynamics of coarse grained polystyrene melts — •Dominik Fritz[1], Vagelis A. Harmandaris[1], Dirk Reith[2], Nico F. A. van der Vegt[1], and Kurt Kremer[1] — [1]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — [2]Fraunhofer-Institut für Algorithmen und Wissenschaftliches Rechnen, Schloss Birlinghoven, 53754 St. Augustin, Germany

Polymers show characteristic properties in a wide range of time scales. To access longer time scales in simulations, purely atomistic simulations are far too expensive to perform. The mesoscopic description of polymers allows to exceed the computational limitations of atomistic simulations. Following a systematic procedure one coarse grains atomistic polymer models into mesoscopic models, which cover time scales larger by several orders of magnitude. By reinserting details into systems, simulated with the mesoscopic model, we get well-equilibrated atomistic systems of high molecular weight.

In this contribution, we study coarse grained models of atactic polystyrene and compare its static and dynamic properties to atomistic simulation data. While static properties are used to develop coarse grained force fields, we look especially at aspects of the time scales in atomistic and mesoscopic simulations. We investigate mapping factors between dynamic properties, e.g. diffusion constants, in atomistic and mesoscopic melt simulations and their dependence on chain length.

CPP 34.47 Thu 17:00 Poster A

Microdomain Dynamics in Thin Films of Blockcopolymer Melts with Highly Ordered Cylinder Morphology — •Peter Fey, Christian Riesch, Sabine Rehse, Nicolaus Rehse, and Robert Magerle — Chemische Physik, TU Chemnitz, 09107 Chemnitz

We study a polystyrene-*block*-polybutadiene copolymer melt which forms cylinders in the bulk. With a shearing device based on a rubber stamp large areas of cylinders oriented parallel to the surface are produced in films of a thickness equivalent to one or two cylinder layers. After alignment, the film surface is imaged with tapping mode atomic force microscopy. It allows *in-situ* observation of the polymer melt during annealing at high temperatures ($\approx$ 100 - 120°C). The fluctuations of the orientation and width of cylinders is quantified using image processing algorithms, such as local Fourier transformations. Our goal is to achieve a better understanding of microdomain shape fluctuations in thermal equilibrium. Specimens with different degree of alignment are used to study the influence of defects on the observed dynamics.

CPP 34.48 Thu 17:00 Poster A

Logarithmic chain-exchange kinetics of diblock copolymer micelles — Reidar Lund[1,2], Lutz Willner[1], •Jörg Stellbrink[1], and Dieter Richter[1] — [1]IFF, Forschungszentrum Jülich, D-52425 Jülich — [2]Donostia International Physics Center, 20018 San Sebastián, Spain

We present a study of equilibrium chain-exchange kinetics of a well-defined model system for starlike PEP-PEO micelles in water/DMF mixtures [1, 2]. In this study we used time resolved small angle neutron scattering (TR-SANS) technique employing a particular H/D labeling scheme. This technique is perfectly suited for determination of exchange kinetics in equilibrium as, unlike other techniques,virtually no chemical or physical perturbations are imposed on the system.

The exchange kinetics crucially depends on the interfacial tension γ. By variation of γ the rate could be tuned over a wide time scale spanning from milliseconds to infinity. The results show that the kinetics follows a logarithmic time dependence [3] in sharp contrast to theory where single exponential behavior is predicted [4]. The logarithmic time dependence hints towards strongly coupled chain dynamics within the micellar cores induced by geometrical constraints. The same feature has been found for two other micellar systems confirming a general feature of exchange kinetics of block copolymer micelles.

[1] R. Lund et al., *Macromolecules*, **37**, 9984-9993, 2004.

[2] M. Laurati et al., *Phys. Rev. Letters*, **94**, 195504, 2005.

[3] R. Lund, et al., *Phys. Rev. Letters*, **96**, 068302, 2006.

[4] A. Halperin and S. Alexander, *Macromolecules*, **22**, 2403, 1989.

CPP 34.49 Thu 17:00 Poster A

Self Assembly of Block Copolymer Micelles — •Michael Ströbl, Gerald Johannes Schneider, Jörg Stellbrink, Jürgen Allgaier, and Dieter Richter — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

Amphiphilic diblock copolymers play a crucial role in basic research as well as in applied science. In aqueous solution these diblock copolymes form micelles, which structure depends on the interfacial tension between the hydrophobic block and the selective solvent.

Using recently synthesized poly(alkyleneoxide)-poly(ethyleneoxide) block copolymers (PAO-PEO) the variation of the interfacial tension can now be achieved by changing the monomer of the hydrophobic block but keeping the same solvent, i.e. water. In the homologue series propyleneoxide (PPO), butyleneoxide (PBO), hexyleneoxide (PHO), and octyleneoxide (POO) the hydrophobicity increases continuously due to the growing aliphatic side group.

We present the results of static light scattering experiments and small angle neutron scattering experiments on the samples mentioned above.

CPP 34.50 Thu 17:00 Poster A

Multiple-quantum NMR study of entangled polymer melt dynamics — •Fabian Vaca Chavez and Kay Saalwachter — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik; Friedemann-Bach-Platz 6, D-06108 Halle (Germany)

Entangled polymers melts exhibit a variety of dynamic processes covering a wide range of time scales, starting form the fast segmental reorientation in the picoseconds scale up to the diffusive and cooperative motions in the range of seconds. NMR is a powerful tool to study molecular dynamics due to its sensitivity to different molecular motions. In particular, multiple quantum (MQ) NMR emerged a few years ago as a new and robust tool to study polymer chain dynamics [1]. This technique yields quantitative information in particular on chain ordering, i.e., on entanglement effects and crosslink densities, and on the timescale of chain motion. In this work, we apply MQ NMR to linear poly(cis -1,4-isoprene) and poly(dimethyl siloxane) over suitable ranges of well defined molecular weight and temperature, in order to establish the dynamic regimes predicted by the tube model, and obtain in in-depth comparison of the entangled dynamics of these polymers. The data is analyzed by establishing simple scaling laws [1], and full analytical expressions based on a correlation function which explicitly includes the Rouse and reptation dynamics [2].

[1] R. Graf, A. Heuer, H.W. Spiess, *Phys. Rev. Lett.*, **80**, 5738-5741 (1998).

[2] K. Saalwachter, A. Heuer, *Macromolecules*, **39**, 3291-3303 (2006).

CPP 34.51 Thu 17:00 Poster A

Polyelectrolyte-Compression Forces between Spherical DNA Brushes — •Kati Kegler[1], Martin Konieczny[2], Gustavo Dominguez-Espinosa[1], Christof Gutsche[1], Matthias Salomo[1], Friedrich Kremer[1], and Christos N. Likos[2] — [1]Institute for Experimental Physics I, University of Leipzig, Linestr. 5, D-04103 Leipzig, Germany — [2]Institute for Theoretical Physics II: Soft Matter, Heinrich-Heine-Universität Düsseldorf, Universitätsstr. 1, D-40225 Düsseldorf, Germany

Optical tweezers are employed to measure the forces of interaction between a single pair of DNA-grafted colloids in dependence of the molecular weight of the DNA-chains, and the concentration and valence of the surrounding ionic medium [1]. The resulting forces are short-range and set in as the surface-to-surface distance between the colloidal cores reaches the value of the brush height. The measured force-distance dependence is analyzed by means of a theoretical treatment based on the compression of the chains on the surface of the opposite-lying colloid. Quantitative agreement with the experiment is obtained for all parameter combinations. [2]

[1] K. Kegler, M. Salomo, and F. Kremer, PRL 98, 058304 (2007)

[2] Kati Kegler, Martin Konieczny, Gustavo Dominguez-Espinosa,Christof Gutsche, Matthias Salomo, Friedrich Kremer, and Christos N. Likos submitted to PRL

CPP 34.52 Thu 17:00 Poster A

Static and dynamic properties of Polyelectrolytes — •Jens Smiatek and Friederike Schmid — Fakultät für Physik, Condensed Matter Theory, Universität Bielefeld, 33615 Bielefeld, Germany

We study the dynamics of charged macromolecules in salt solutions, taking full account of the electrostatic and the hydrodynamic interactions.

The polyelectrolyte is modeled by a simple coarse-grained bead-spring model which is embedded in free solution. All particles are simulated by Dissipative Particle Dynamics and we use the freely available software package ESPResSo.

Special interest is spent on the dynamic and static properties of polyelectrolytes like the structure factor and the single monomer displacement. All results will be carefully analyzed in the light of existing theories.

CPP 34.53 Thu 17:00 Poster A

Polypyrrole Nanowires Grown from Polyelectrolyte Single Molecules — •Vera Bocharova[1], Anton Kiriy[1], Hartmut

Vinzelberg[2], Ingolf Moench[2], and Manfred Stamm[1] — [1]Leibniz Institute of Polymer Research Dresden, Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research, Dresden, Germany

Low-dimensional nanostructures of conductive polymers have attracted a great interest as building blocks for future miniatuarized nanoelectronic devices and highly sensitive chemical or biological sensors. We have developed a template method to grow continuous highly conductive polypyrrole (Ppy) nanovires (NWs) of variable diameter by polymerization of pyrrole from individual adsorbed polystyrene sulfonic acid (PSA) molecules. [Bocharova, V. Kiriy, A.; Vinzelberg, H.; Mönch, I.; Stamm, M. Angew. Chem. 2005, 117, 6549] The DC conductivity of individual Ppy NWs is not linearly dependent on their diameter. It is likely due to of granular structure of the NWs and a percolation-like conductivity reflecting a transition from the 1D to 2D and then to 3D-percolation networks of grains resulting into increase of the conductivity up to typical Ppy bulk conductivity. We found that the conductivity decreases with decreasing of temperature, as typical for semiconductors. The conductivity can be described using variable-range hopping model. According to this model the transition from 2D to 3D-percolation network of spherical grains was found.

CPP 34.54 Thu 17:00 Poster A

Influence of solvent and counterion on the effective charge and size of polyelectrolytes — •Ute Böhme and Ulrich Scheler — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, D-01069 Dresden, Germany

The effective charge of polyelectrolytes in mixtures of organic solvents and water is primarily governed by the permittivity. Decreasing the dielectric constant leads to stronger charge- charge interaction on the polyelectrolyte resulting in enhanced counterion condensation and thus reduced effective charge. A combination of diffusion and electrophoresis NMR is applied to determine the effective charge of polyelectrolytes with different monovalent counterions in polar solvents adjusting permittivity by water content [1,2].

In solvents with high water fraction the charge decreases linearly with the permittivity while in mixtures with low water content the effective charge and size of the polyelectrolyte drops dramatically depending on the counterion. Reduced repulsive interactions between the charges along the chain lead to a more compact conformation of the polyelectrolyte.

[1] U. Scheler in H.S. Nalwa (ed.): Handbook of Polyelectrolytes and their applications, American Scientific Publishers (2002), Vol.2

[2] U. Böhme, U. Scheler, J. Colloid Interface Sci., 309, (2007), 231.

CPP 34.55 Thu 17:00 Poster A

Phase behavior of polyelectrolyte multilayer investigated by thin film calorimetry — •Heiko Huth[1], Renate Müller[2], Andreas Fery[3], and Christoph Schick[1] — [1]Universität Rostock Institut für Physik, Universitätsplatz 3, 18051 Rostock — [2]MPI für Kolloid- und Grenzflächenforschung, Am Mühlenberg, 14424 Potsdam — [3]Universität Bayreuth Physikalische Chemie II, Universitätsstr. 30, 95447 Bayreuth

Polyelectrolyte multilayer can be easily assembled using spraying or dipping of the different polyelectrolytes [1]. The thickness of the produced layers (nanometer range) is well controlled by the preparation conditions. Only a few methods are available for dynamic investigations, as afm for mechanical properties [2].

AC-chip calorimetry is used as a very sensitive tool for calorimetric investigations of such thin films as demonstrated for thin polymeric films [3]. To investigate the phase behavior of polyelectrolytes the humidity is used as a new parameter in addition to temperature for calorimetry. First measurements with the modified calorimeter for the PSS/PDADMAC polyelectrolyte multilayer system are shown. Further extensions of the calorimeter for better understanding of the phase behavior are discussed.

[1] Decher, G. and J.D. Hong, Phys. Chem. Chem. Phys., 1991. 95(11): 1430.

[2] Mueller, R., et al. Macromolecules, 2005. 38(23): 9766.

[3] Huth, H., Minakov, A. A., Schick, C., J. Polym. Sci. B Polym. Phys. 2006 44: 2996.

CPP 34.56 Thu 17:00 Poster A

Forces of interaction between polyacrylic acid brushes as measured by optical tweezers — •Gustavo Dominguez-Espinosa[1], Alla Synytska[2], Astrid Drechlser[2], Christof Gutsche[1], Friedrich Kremer[1], Petra Uhlmann[2], and Manfred Stamm[2] — [1]Institute of Experimental Physics I, Leipzig University, Linnéstr. 5, 04103, Leipzig, Germany — [2]Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, 01069, Dresden, Germany

The forces of interaction between polyacrylic acid brushes grafted on two separated silica colloids are measured by Optical Tweezers (resolution of the forces 0.5 pN and resolution in position 3 nm). The interaction potential of the polyacrylic acid brushes is determined in dependence of the pH, ion concentration and valence of the surrounding medium. Scaling of the brush thickness with the power of the ionic strength is found in qualitative agreement with the theoretical predictions. The observed increase in the brush thickness with the increasing pH is attributed to the electrostatic repulsion caused by dissociation of the polyacrylic acid.

CPP 34.57 Thu 17:00 Poster A

Influence of preparation conditions on lateral and vertical surface structure of polyelectrolyte multilayers — •Matthias Cornelsen, Stephan Block, Manesh Gopinadhan, and Christiane A. Helm — Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17487 Greifswald, Germany

Polyelectrolyte multilayers from PAH and PSS are formed at different ion concentrations and temperatures. If the electrostatic force is screened (i.e. the ion concentration exceeds 0.05 M), then the film thickness increases on the rise of both temperature and salt concentration. However, for each salt concentration there is a maximum temperature up to which stable films can be formed. If films from temperatures 40 to 5 K below this maximum temperature are compared, one finds with X-ray reflectivity that the film/air roughness increases (from 1 to 4.5 nm) on approach to the maximum temperature. Also, with AFM a surface coarsening is observed on the scale of 150 to 300 nm. Furthermore, the average distance between height maxima is measured, which changes depending on preparation conditions from 15 to 30 nm. These maxima may be attributed to coils or parts of coils of single chains.

CPP 34.58 Thu 17:00 Poster A

Water incorporation in poylectrolyte multilayers: Hofmeister effect? — •Oxana Ivanova[1], Olaf Soltwedel[1], Manesh Gopinadhan[1], Jens-Uwe Günther[1], Matthias Cornelsen[1], Roland Steitz[2], and Chrstiane A. Helm[1] — [1]Institut für Physik,Ernst-Moritz-Arndt Universität,Felix-Hausdorff-Straße 6, 17489 Greifswald,Germany — [2]Hahn-Meitner Institut, Glienicker Straße 100, D-14109 Berlin, Germany

The Hofmeister effect - the effect of salt on the hydrophobic effect - on the formation of polyelectrolyte multilayers is studied. Films are prepared while varying the preparation temperature T and the countercation (1 M XCl). For characterization, X-ray and neutron reflectivity are used. Selectively deuterated polyanion layers lead to at least two superstructure peaks. The PAH/PSS bilayer thickness is independent of the kind of salt and increases on temperature rise. Yet, at low T the amount of bound water depends strongly on the position of the cation in the Hofmeister series ($Cs^+ < Ka^+ < Na^+$). The internal roughness is 30-40 % of the bilayer thickness; it increases to up to 60% at high T. The temperature at which the roughening starts is a function of the countercation (ca. 50°C for NaCl, ca. 40°C for KCl and ca. 30°C for CsCl). It appears that the temperature effect - which is attributed to the melting of the first-shell water on temperature rise - is promoted by the countercations as predicted by the Hofmeister series. The effect is subtle; it manifests itself as an increased internal roughness, a loss of bound water and a downshift of the roughening temperature - whereas the thickness of the deposited bilayer is not affected.