CPP 13: POSTERS Polymer Physics

Time: Tuesday 14:00–16:30 Location: P3

CPP 13.1 Tue 14:00 P3

Automatic mapping of WAXS fiber patterns and its application: Crystallization mechanisms in polypropylene —
•Norbert Stribeck[1], Ulrich Nöchel[1], and Sérgio S. Funari[2] — [1]Universität Hamburg, Institut TMC, 20146 Hamburg, Germany — [2]HASYLAB c/o DESY, 22603 Hamburg, Germany

In time-resolved WAXS studies thousands of patterns are recorded that must be mapped into reciprocal space and evaluated for structure evolution analysis. Crystallographers refine an approximation, but this takes time. The exact solution [1] for fiber orientation with respect to the detector plane is found. Then an automatic mapping and evaluation algorithm [2] is devised. For oriented polypropylene it returns weight crystallinities and crystallite sizes for two sets of crystallites that are differently oriented (c, a^*). The method is applied in a study of crystallization mechanisms by WAXS [3] and SAXS [4]. At shallow quench we observe (1) decomposition of the amorphous melt, (2) a nucleation regime of several minutes in which crystallinity stays below 1% (latency period), (3) a growth regime with rapid growth of crystallinity. Begin and length of the latency period are different for c- and a^*-set and vary as a function of undercooling.

[1] Stribeck Acta Cryst. (2009), doi:10.1107/S0108767308029772
[2] Stribeck *et al.* J. Appl. Cryst., submitted Sept 2008
[3] Stribeck *et al.*, Macromolecules, submitted Nov 2008
[4] Stribeck *et al.*, Macromolecules (2007), 40(13), 4535-4545

CPP 13.2 Tue 14:00 P3

Dipole moment dependent investigation of Surface Relief Grating formation on azobenzene polymer thin films —
•Padmanabh Veer[1], Ullrich Pietsch[1], Paul Rochon[2], and Marina Saphiannikova[3] — [1]Department of Solid State Physics, University of Siegen, ENC, 57068, Siegen, Germany — [2]Department of Physics, Royal Military College, Kingston, Ontario, Canada K7K5L0 — [3]Leibniz Institute of Polymer Research, 01069, Dresden, Germany

The formation mechanism of surface relief gratings (SRGs) was studied in the context of dipole moment of the azobenzene material with respect to time and temperature dependent measurements. The orientation mechanism of chromophore as an initiative to the grating formation was studied insitu using continuous and pulse like exposure techniques at various temperatures upto the glass transition temperature (TG) of the respective polymer material. The results obtained for high dipole moment pDR1M and low dipole moment pMEA were compared in terms of the rate of the grating formation and related to the quantities as relaxation of the chromophores in the absence of the inscribing light and induced stress due to the chromophore orientation. The parameters obtained from the simulation data can be well explained in the frame of the viscoplastic approach. The deformation caused by the light induced movement of the azopolymer chains has found to alter the mechanical properties of the polymer material.

CPP 13.3 Tue 14:00 P3

Dielectric Spectroscopy and Rheology on Different Poly(alkylene oxide)s —
•Christine Gerstl[1], Gerald Johannes Schneider[1], Wim Pyckhout-Hintzen[1], Jürgen Allgaier[1], Angel Alegria[2], Juan Colmenero[2,3], and Dieter Richter[1] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Centro de Fisica de Materiales, Apartado 1072, 20080 San Sebastian, Spain — [3]Donostia International Phyics Center, Apartado 1072, 20080 San Sebastian, Spain

Poly(alkylene oxide)s (PAOs) form a homologous series of type-A polymers with side groups of varying length. Since the PAOs poly(ethylene oxide) and poly(propylene oxide) are known for a long time and have been studied extensively, the higher homologues are ideally suited to probe the influence of side chains on the dynamics of a polymer.

We will present the results of dielectric and rheologic measurements on poly(butylene oxide), poly(hexylene oxide) and poly(octylene oxide), having side groups of $(CH_2)CH_3$, $(CH_2)_3CH_3$, and $(CH_2)_5CH_3$ respectively. The relaxation of the whole polymer chain as well as the segmental dynamics will be discussed in terms of different models and compared to existing results.

CPP 13.4 Tue 14:00 P3

Synthesis and characterization of metallopolymer nanocomposites based on PAN —
•Marat Bulatov[1], Ullrich Pietsch[2], and Tobias Panzner[2] — [1]Astrakhan State University, 414056 Astrakhan, Russia — [2]Universität Siegen, 57072 Siegen, Germany

Conductive polymers are widely used in manufacturing of electrodes of various technical application and for use in micro- and nanoelectronics. Also the application of conductive polymers for data storage and photoconversion is very challenging. The aim of the present work is investigation and optimization of the preparation technology for composites based on polyacrylonitrile (PAN). In particular we have prepared nanocomposites of iron (Fe/PAN) and nickel (Ni/PAN). The samples have been produced by means of the infrared heating method with various Fe and Ni concentrations. Structurual characterisation was performed by X-ray powder diffraction, X-ray fluorescence analysis, IR and Raman spectroscopy, as well as by synchrotron scattering and EXAFS techniques. It was observed that after synthesis the nickel atoms have formed crystallized nanoclusters with a size smaller than 30 nm. After analysis of the IR-spectra and literature data we can assume that the iron atoms are distributed within the the polymer matrix and most likey form iron polyacrylate (FePAcr). Finally the structure of nanocomosites is correlated to the magnetic properties of the obtained samples. Acknowledgement: M.Bulatov thanks DAAD for financial support.

CPP 13.5 Tue 14:00 P3

Light induced lattice expansion in azopolymer films —
•Sebastian Kramer, Padmanabh Veer, and Ullrich Pietsch — Department of Solid State Physics, University of Siegen, ENC, 57068, Siegen, Germany

Light induced lattice expansion of azopolymer films was observed under homogeneous illumination with polarized light of 514nm of about 1W. The polymer film made from pDR1M was irradiated parallel to the surface normal. The light induced deformation effects were probed using a low power He-Ne laser of wavelength (λ=633nm) at a fixed reflection angle of about 63 degree and recorded using a pair of photodiodes. Straight after switching the actinic light on the intensity of the probe laser shows a sudden jump followed by an oscillation behavior damped out as function of time. Evaluated in terms of Fresnel equations the sudden increase and the oscillations can be related to the change in the refractive index and an increase of film thickness under light illumination. Considering the Gaussian profile of the laser beam the evaluated increase in film thickness reaches a value of several 100nm in centre and decreases respectively towards the borders. The behavior can be explained in terms of light-induced visco-elastic flow.

CPP 13.6 Tue 14:00 P3

Quantitative analysis of block copolymer microdomain dynamics —
•Christian Riesch, Eike-Christian Spitzner, and Robert Magerle — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

Microdomain ordering in a thin film of a cylinder-forming diblock copolymer is observed during vapour annealing by in situ atomic force microscopy. The ordering process is observed with high temporal resolution of $\sim$ 60 s/frame over several hours. The domain coarsening in the resulting image series is analysed using local and global measures of order. We compute orientation maps, local curvature and correlation lengths; furthermore the temporal evolution of individual defects is tracked. The experimental results are compared with the microdomain dynamics observed in cell dynamics simulations of a similar system. We investigate the influence of film thickness and polymer-substrate interactions.

CPP 13.7 Tue 14:00 P3

Micromechanics of thin films of elastomeric polypropylene —
•Mechthild Franke and Robert Magerle — Chemische Physik,TU Chemnitz, 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. We stretch $\sim$ 1 μm thick films stepwise up to 100% and observe the changes in shape, orientation, and morphology of crystalline regions in situ with scanning force microscopy. We

find heterogeneous deformations on length scales smaller than 2 μm. On larger length scales the deformation is homogeneous. Branching points of epitaxial grown branches on mother lamellae are very rigid and do not deform up to strains of $\sim 40\%$. Reversible bending of single lamellae is also observed. On stretching, some lamellae break into fragments which upon further stretching break into smaller, only 10 nm large, blocks. Less frequently, we observe strain induced melting and crystallization. Our setup allows for a number of novel experiments. For instance, cyclic loading could reveal processes on the nanometer scale leading to fatigue behavior of the specimen.

CPP 13.8 Tue 14:00 P3

Investigation of Laser Heating Effects on Polymerfilms — •Ralf St. Kappes[1,2] and Jochen S. Gutmann[1,2] — [1]Joh.-Gutenberg University, Mainz, Germany — [2]Max-Planck-Institute for Polymer Research, Mainz, Germany

With Laser heating it is possible to deposit large amounts of energy in short time scales to a small region and by that create far from equilibrium conditions. In that context, we applied a NIR-laser pulse of microsecond duration to a thin PS-Film, doped with a dye for energy conversion, observing the spectrum of the thermal radiation. Therefore we built up an optical detection system using interference filters and a microsecond-gated camera as detector. By then fitting Planck law to the spectral curve we were able to obtain the temperature and could show that the peak temperature is in the order of 1000 K, with a non-linear dependence of the dye concentration. Furthermore with this approach it was possible to obtain a temperature-time-profile and investigate the behaviour of the thin film system under such extreme conditions.

CPP 13.9 Tue 14:00 P3

Dynamical properties of chain molecules in confinements and in variation of system properties: model of DNA segregation — •Ron Dockhorn[1,2] and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research Dresden, D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany

Large chain molecules are studied and simulated in various conditions such as restricted geometries, interaction potential and solvent quality using the bond fluctuation method. How relaxation time, diffusion and segregation time are related due to strong confinements is analyzed and compared to scaling approaches. The investigations are also focused on the influence of topological constraints such as linear and circular polymers and excluded volume effect in confinements compared with theoretical predictions. The process of duplicating and segregating of chain molecules in cylindrical confinements is examined as a model of prokaryotic DNA during replication. Furthermore the model can be extended to study the influence of condensin, cohesin and topoisomerases in DNA condensation and segregation in eukaryotes.

CPP 13.10 Tue 14:00 P3

Mobility of single polymer chains in thin films by widefield fluorescence microscopy — •Bente Marid Ingeborg Flier and Andreas Zumbusch — Fachbereich Chemie, Universität Konstanz, D-78457 Konstanz

Thin polymer films with a thickness of several tens of nanometers are of high interest both for scientific and industrial applications. The adhesion and interdiffusion properties of such films are affected by the mobility of the polymer chains. In order to probe bulk-obscured heterogenities in the chain mobility we use single molecule fluorescence techniques. For this purpose, single fluorescent molecules are covalently attached as labels to the end of a polymer chain and their motion is observed via fluorescence wide-field microscopy. We use two different approaches to investigate dynamical processes. Rotational diffusion of a fluorophor is observed by defocused imaging. Defocussing the sample under investigation leads to patterns in spatial distribution of the emitted photons which are specific for each orientation of the emission dipole. Analysing the orientational dynamics allows the analysis of rotational diffusion. Translational diffusion, by contrast, can be observed by determining the position of the fluorophors and analysing the trajectories by single particle tracking. We present results of investigations of the dependence of polymer chain mobility on chain length and temperature using both approaches.

CPP 13.11 Tue 14:00 P3

Quantitative analysis of energy dissipation processes during tapping mode atomic force microscopy of soft materials. — •Eike-Christian Spitzner, Christian Riesch, Christian Dietz, and Robert Magerle — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

We aim for a better understanding of the energy dissipation processes during tapping mode atomic force microscopy of soft materials. As model systems we investigate thin films of polystyrene homopolymer and polystyrene-*block*-polybutadiene diblock copolymers. The mechanical properties of the specimen are varied by controlled swelling in chloroform vapor. With an atomic force microscope operated in tapping mode, the energy dissipated between tip and sample, as well as the tip indentation into the polymer film, are determined. Polystyrene and polybutadiene differ in the amount of dissipated energy as well as in the detailed shape of energy dissipation curves as function of amplitude set point. Possible energy dissipation processes causing these differences are discussed.

CPP 13.12 Tue 14:00 P3

Ion transport mechanisms in polymer electrolytes - a molecular dynamics simulation study — •Diddo Diddens[1,2], Andreas Heuer[1,2], and Oleg Borodin[3] — [1]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 30, 48149 Münster, Germany — [2]NRW Graduate School of Chemistry, Corrensstraße 36, 48149 Münster, Germany — [3]Department of Materials Science and Engineering, 122 S. Central Campus Dr, Rm 304, University of Utah, Salt Lake City, Utah 84112-0560

Solid state polymer electrolytes based on poly(ethylene oxide) (PEO) and lithium salts have been intensely studied both experimentally and theoretically and are thus a prototype for technical applications such as batteries or fuel cells. The motion of the ions in such electrolytes is complex due to the amorphous polymer matrix and has not yet been fully understood. In contrast to ceramic ion conductors the host network is not immobile and also contributes to the net transport. We studied both intramolecular and intermolecular ion transport mechanisms by MD simulations of an electrolyte composed of PEO and LiTFSI. Special emphasis was placed on the transfer of ions between different PEO molecules, which is of fundamental relevance for the resulting macroscopic conductivity.

CPP 13.13 Tue 14:00 P3

Polymer phase diagram in ionic liquids — •Daniela Fell[1,2] and Jochen S. Gutmann[1,2] — [1]University of Mainz, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany

We have developed a new, fast and simple method for recording polymer phase diagrams using a normal flatbed scanner. The synchronization of the scanner and a temperature control unit allows us to automatically heat our setup in well-defined steps and then automatically scan. In one measurement series we are able to examine up to 80 different polymer concentrations. With this setup we are detecting the change of the cloudiness of a polymer in an ionic liquid. The obtained pictures are automatically analysed and the results are transferred to a single phase diagram.

With the help of this fast and automated method we have recorded phase diagrams of polymethylmethacrylate (PMMA) of different molecular weights in the room-temperature ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate ([bmim][PF6]).

CPP 13.14 Tue 14:00 P3

Patterning of surface immobilized ATRP starter — •Sebastian G.J. Emmerling and Jochen S. Gutmann — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany

Patterning of silanes on silicon surfaces by photolithography or electron beam lithography has become a routine technique. Photolithography however involves several steps and therefore can be time-consuming, as it is the case in electron beam lithography. In contrast to this, we have developed a method to pattern an ATRP-starter that is immobilized on a silicon surface via a silane group with the use of an inject-printer. Since the ATRP-starter (4-(Chlorodimethylsilyl)-2-methylbutan-2-yl 2-bromo-2-methylpropanoate) contains a hydrolytically labile bromoester functionality, we printed sulphuric acid to cleave the molecule at this point. The remains on the surface then contain no longer a bromo-functionality and thus are inactive in ATRP. Subsequently PMMA brushes grew then selectively in the areas, which had not been in contact with sulphuric acid. Imaging ellipsometry allowed to measure site specific the film thickness. Depending on the concentration of the plotted sulphuric acid, we were able to tune the density of starter molecules in the plotted region. Given that in ATRP

all chains grow to the same length, the density determines the thickness of the produced polymer film, which we were able to observe. The advantage of this technique is that large areas can be patterned quickly in just one step, while the smallest features generated thus far were single droplets the size of 100 to 200 micrometer.

CPP 13.15   Tue 14:00   P3

Quantum dot synthesis on thin polymer films — •Jannis Ochsmann[1,2] and Jochen Gutmann[1,2] — [1]Max-Planck Institute für Polymerforschung, 55128 Mainz, Germany — [2]Universität Mainz, 55099 Mainz, Deutschland

Thin polymer films of asymmetric diblock copolymer of polystyrene and poly(ethylene oxide), PS-b-PEO, were spin-coated on glass substrate. The conditions were optimised to obtain cylindrical PEO microdomains normal to the surface1. The obtained PEO domains were swollen by immersing the copolymer film in an acidic thioacetamide solution. Heating the film induces a hydrolysation reaction of the thioacetamide and S2-ions were obtained inside the PEO microdomains. By this means, we created a localized S2-ions source in the film. Immersing the swollen film into a solution of CdCl2, leads to an reaction between the S2-ions and the Cd2+ions at the film/water interface to form CdS quantum dots. The effect of the concentration of thioacetamide, CdCl2, the temperature and pH is investigated with AFM, X-ray reflectivity and UV/Vis spectroscopy.

1Kim, D. H., S. H. Kim, et al. (2004) Nano Letters 4(10): 1841-1844

CPP 13.16   Tue 14:00   P3

Structure-property relationship in minor ampullate spider silk as studied by combined mechanical and time-resolved polarized FTIR spectroscopy — •Roxana-Giorgiana Ene, Periklis Papadopoulos, and Friedrich Kremer — Institut für Experimentelle Physik I, Leipzig, Germany

Simultaneous FTIR and mechanical measurements are employed in order to explore the relation between macroscopic and microscopic properties, in spider silk[1].Minor ampullate has been studied because although its chemical structure is similar with major ampullate,their mechanical properties differ considerably[2].The way the different nanocrystalline building blocks are interconnected is investigated by stretching the sample. Mechanical studies on minor ampullate silk show that the stiff crystalline domains are connected in series with the amorphous chains and that the mechanical field inside the fiber is uniform[3]. The results reveal oriented crystals interconnected by prestrained chains. It is shown that minor ampullate can be described by the same model[2] as for major. The prestress is significantly lower, explaining the lower modulus, while the toughness is similar. References: [1]P.Papadopoulos, J.Sölter, F.Kremer;Eur.Phys.J.E:Soft Matter 24,193(2007) [2]P.Papadopoulos, J.Sölter, F.Kremer;in press Colloid Polym.Sci(2008) [3]P.Papadopoulos, R.G.Ene, I.Weidner, F.Kremer (in preparation)

CPP 13.17   Tue 14:00   P3

Polymer blends and diblock copolymer melts in external electric fields — •Ilja Gunkel[1] and Semjon Stepanow[2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, 06099 Halle, Germany

We generalize the statistical mechanical description of low molecular liquid systems in external electric fields in the E-ensemble at constant potential [1] to polymer blends and diblock copolymer melts. The anisotropic part of the segment polarizability results in a change of the polymer shape from a Gaussian coil to an ellipsoid. The effective binary interactions between the segments, which we have calculated to the quadratic order in the segment polarizabilities, are attractive in the ensemble at fixed potential, and result in an upward shift of the critical temperature in phase transitions in these systems. We have generalized the Flory-Huggins free energy for polymer blends in an electric field in both the E- and the E0-ensembles (constant charges). The collective structure factor for diblock copolymer melts is computed by taking into account the anisotropic parts of the segment polarizabilities as well as the effective binary interactions. We also computed the dielectric permittivity of the diblock copolymer melt in the vicinity of the order-disorder transition. The results of the statistical mechanical treatment of diblock copolymer melts are compared with the existing phenomenological approaches for these systems.

[1] S. Stepanow and T. Thurn-Albrecht, submitted, preprint http://arxiv.org/abs/0810.1881

CPP 13.18   Tue 14:00   P3

Adsorption of nano-particles on polymer brushes — •Huilan Zhang[1], Holger Merlitz[2], and Jens-Uwe Sommer[1] — [1]Leibniz-Instituts für Polymerforschung Dresden, Germany — [2]Department of Physics, Xiamen University, Xiamen, PRC

We investigate the interaction of nano-particles with polymer brush using molecular dynamics simulations. The adsorption properties of particles and the equilibrium structure of the polymer brush (thickness, monomer density profile, distribution of end monomers) are studied at different grafting densities and temperatures. A stretch-collaps transition is found for the particle-brush complex at a threshold temperature T_0, depending on the particle size and grafting density. At high temperatures, above T_0, due to the dominant excluded volume effect the brush will stretch out and increase the coverage of the particles inside the brush by decreasing the temperature. For temperatures lower than T_0, the increasing contacts between the particles and monomers will drive the brush into a compact brush-particle complex. We found a maximum particle number trapped in the brush and a maximum loading capacity of the brush for a given brush-particle configuration. Additionally, the influence of particle size and chain length of polymer on the behavior of the brush-particle complex has been studied.

CPP 13.19   Tue 14:00   P3

Infrared Transition Moment Orientational Analysis on Liquid Single Crystal Nematic Elastomers — •Wilhelm Kossack[1], Periklis Papadopoulos[1], Felicitas Brömmel[2], Heino Finkelmann[2], and Friedrich Kremer[1] — [1]Universität Leipzig, Institut für Experimentelle Physik I, Linnéstr. 5, 04103 Leipzig — [2]Albert-Ludwigs-Universität Freiburg, Institute for Macromolecular Chemistry, Stefan Meier-Str. 31, 79104 Freiburg

Liquid *Single* Crystal Nematic Elastomers (LSCNE) form a novel class of materials combining the properties of liquid crystals with elastomeric networks and in which the crystalline order is extended to and stabilized on a macroscopic scale ($\sim$cm^2). In order to determine mean orientation and molecular order parameter of the different molecular moieties (mesogen, polymer backbone, etc.) IR-Transition Moment Orientational Analysis (IR-TMOA) is employed. This technique takes advantage from the specifity of the IR spectral range. Based on the measurements of the transmission dependence of polarization and an intentionally adjusted inclination of the sample numerical analysis of Fresnel-equations enables one to determine seperately real *and* imaginary part of the refractive index n^*. From that mean orientation and molecular order parameter of the molecular moieties, represented by different absorption bands, are deduced. As further refinement the sample can be mechanically stretched during the IR measurements. By that the microscopic response to macroscopic excitation can be unraveled and phenomena like elastic memory effects and the phase relationships in reorientation of the molecular units can be traced.

CPP 13.20   Tue 14:00   P3

Temperature-resolved structures and kinetics of deswelling in PNIPAM hydrogels and solutions — •Andreas Meier-Koll[1], Anastasia Golosova[1], Joseph Adelsberger[1], Weinan Wang[1], Peter Busch[2], Vitaliy Pipich[2], Christine M. Papadakis[1], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department E13, Garching — [2]JCNS at FRM II, Garching

The deswelling behavior as well as its kinetics of highly concentrated aqueous poly(N-isopropylacrylamide) (PNIPAM) solutions are investigated with small angle neutron scattering (SANS) and are discussed in terms of spinodal decomposition. The phase transition is shown to be of second order. After a temperature jump from the swollen to the deswollen state, three different time regimes of the decomposition process are observed: In the early stage, small fluctuations of the density are reinforced by the negative curvature of the Gibbs free energy, which lead to a negative diffusion coefficient and an exponential increase of the scattering intensity. Within this time, well-defined interfaces between both species are formed. The corresponding strong forward scattering can be described by a Porod behavior. The coarsening in the intermediate and late stage manifests itself in a decrease of the forward scattering intensity which follows a power law behavior with an exponent below 1 in the intermediate, whereas an unusual exponent above 1 is observed in the late stage.

CPP 13.21   Tue 14:00   P3

ESPResSo++ - Extensible Simulation Package for Research on Soft Matter Systems — •Axel Arnold[1], Thomas Brandes[1], Dirk Reith[1], Anton Schüller[1], Jonathan Halverson[2], Olaf

Lenz[2], and Torsten Stühn[2] — [1]Fraunhofer institute SCAI, St. Augustin, Germany — [2]MPI for polymer research, Mainz, Germany

We present the simulation package ESPResSo and its successor, ESPResSo++, which is currently under development. ESPResSo is designed to be an extensible and flexible tool to perform Molecular dynamics studies on coarse grained soft matter models in a parallel environment. Being developed by the MPI for polymer research in collaboration with the Fraunhofer institute SCAI, the software is particularly suited for polymer systems, but has also been successfully applied to other systems such as colloids or lipid membranes.

Its particular strengths are a flexible script interface, state-of-art algorithms for the calculation of interactions and an extensive set of more than 30 analysis routines. Included algorithms are e.g. RATTLE for constraints, P3M, ELC, MMM1/2D for electrostatics in partially periodic boundary conditions, or Lattice-Boltzmann for hydrodynamics. New interactions can be easily added even by unexperienced users due to simple interfaces, providing an easy to use platform to implement and test new algorithms. Nevertheless, the code is parallelized and has been shown to run on up to 1024 processors.

ESPResSo is maintained as an open-source project, and is used by many users world-wide. For further information, see http://www.espresso.mpg.de.

CPP 13.22 Tue 14:00 P3
MD Simulations of Sheared Polymer Brushes with Explicit Solvent — •Andre Galuschko, Torsten Kreer, and Jörg Baschnagel — Institut Charles Sadron CNRS, 23, rue du Loess, 67034 Strasbourg Cedex 2, 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.[3,4,5]), 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 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.
We compare our simulation results with the same model without explicit solvent. [1] T. Moro, Y. Takatori, K. Ishihara, 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, E.S.G. Shaqfeh, A.P. Gast, *Phys. Rev. Lett.* **78**, 1182 (1997). [5] T. Kreer, M.H. Müser, K. Binder, J. Klein, *Langmuir* **17**, 7804 (2001).

CPP 13.23 Tue 14:00 P3
Polymer-grafted silica nanoparticles: a structural characterization in solution and bulk — •Mathias Meyer[1], Eike Hübner[1], Wim Pyckhout-Hintzen[1], Jürgen Allgaier[1], Jörg Stellbrink[1], Aurel Radulescu[2], Dieter Richter[1,2], and Horst Weiss[3] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich GmbH — [2]Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH — [3]BASF AG Ludwigshafen

In the framework of an EU FP7 propals with coordination by BASF, nanoparticles basing on organo-modified commercial silica particles of definite size are chemically grafted with PS and PB chains of different length and graft density. They serve as model filler and viscosity modifier if blended with linear matrices. In a combination of SANS, SAXS, DLS and rheology measurements we have characterized the silica nanoparticles with and without grafted polybutadiene and polysyrene in solution and in the blend. The focus of the investigation is on the radial density profile in the various combinations of graft density, chain length and type of the graft as well as the matrix being ideally short-chained i.e. solvent or of intermediate length compared to the grafts. The experiments take profit from the different scattering contrasts and partial labeling. Methods of synthesis i.e. grafting from and grafting to are compared.

CPP 13.24 Tue 14:00 P3
Surface plasmon assisted reversal switching nanolithography — •Tobias König and Svetlana Santer — Department of Microsystems Engineering (IMTEK), University of Freiburg

We have recently suggested that it should be possible to move or repo-

sition strongly adsorbed nano-objects with relative ease, in large number and simultaneously. The essential idea is not to put more effort in fighting against the prevailing surface forces but rather to utilize them - in clear contrast to current techniques of nano-manipulation with atomic force microscopy (AFM) [S. Santer et. al, Advanced Materials 18, (2006) 2359-2362]. Here we present photosensitive polymer thin films [T. Seki, Chemical Society of Japan 80, (2007) 2084-2109] with integrated optically active elements which are supposed to support and steer the response of polymer films to external UV-illumination by acting as nano-scale antennas. For this, we are going to exploit the properties of surface plasmons excited within metal gratings during UV irradiation at a certain wavelength. The resulting intensity distribution leads to a corresponding change in topography that can be changed back to its initial state by irradiating with a different wavelength. In contrast to direct illumination with UV-interference patterns, the use of plasmon interference from metal gratings will allow to generate intensity variation and thus topographical structures below the diffraction limit. This opens up several new possibilities in the field of nano-manipulation discussed in this work.

CPP 13.25 Tue 14:00 P3
Multistage switching in bent-core smectic liquid crystal: Experiment and theory — •Stephan Stern, Alexey Eremin, and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg

We describe a novel type of switching behavior in a series of homologuous bent-core liquid crystal compounds in external dc electric fields. This kind of switching is distinguished by the occurrence of an intermediate field-induced ferrielectric state between an antiferroelectric ground state (off-state) and a ferroelectric on-state. Here we present the results of Second-Harmonic-Generation (SHG) experiments on those compounds, propose a structure for the ground state and the field induced states and develop a simple Ising-type model which can account for the unusual switching behaviour.
S. Findeisen et al., EPJ (2008)

CPP 13.26 Tue 14:00 P3
Toroidal Microcavities Produced by Self-Rolling of Strained Polymer Bilayer — •Kamlesh Kumar[1], Valeriy Luchnikov[2], and Manfred Stamm Stamm[1] — [1]Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, 01069 Dresden, Germany — [2]Institute de Chimie des Surfaces et Interfaces, rue Jean Starcky 15, 68057 Mulhouse, France.

We have demonstrated the fabrication of microtoroids by self-rolling of crosslinked thin strained bilayer polymer films, composed of polystyrene (PS)/poly (4-vinyl pyridine) (P4VP) and released in controllable manner from a solid substrate. The toroids formation proceeds from a circular opening in the film made by photolithography or by mechanical scratching followed by immersion of patterned sample in 2 wt % dodecylbenzene sulfonic acid solution (DBSA). DBSA forms supramolecular complexes with pyridine rings of P4VP and increases the specific volume of the polymer. Since the PS layer is neutral in this solution, bilayer film develops strain due to unequal swelling of polymers in solution of DBSA and hence the film bends and scrolls in order to minimize its free energy. The increasing radius of the toroid causes lateral strain in the film, such that the strain isolines are closed concentric circles centered at the middle of the lithographic window. Furthermore, the kinetics of toroid formation is also studied. The toroids with metallic inner surface are promising for the future research as IR-frequency range resonators.
[1] V. Luchnikov, K. Kumar, M. Stamm, J. Micromech. Microeng. 2008, 18, 035041

CPP 13.27 Tue 14:00 P3
Improving Long Range Order in Block Copolymer based Nanotemplates — •Marcus Böhme, Bhanu Nandan, and Manfred Stamm — Leibniz-Institut für Polymerforschung Dresden, Hohe Str. 6, 01069 Dresden

Thin films of block copolymers and block copolymer based supramolecular assemblies (SMA) are promising candidates for the generation of self assembled templates. One of the biggest challenges in such soft matter systems is the creation of nanostructures which are uniformly ordered on a large scale. In most cases the long range ordering in block copolymer based thin films is either not sufficient for possible applications e.g. in storage technology or can only be achieved with expensive and time-consuming pre-patterning methods (guided self assembly).
It has been shown, that an appropriate treatment with solvent

vapours can improve the ordering in thin films of block copolymers[1] or SMA[2] at least on a scale of a few micrometers. We would like to present our recent results on the improvement of the solvent annealing process and the resulting effects on the long range order in thin films of Poly(styrene-*b*-4-vinyl pyridine) (PS-P4VP) as an example for block copolymer templates and thin films of PS-P4VP with 2-(4-Hydroxyphenylazo)benzoic acid (HABA) as an example of SMA templates. [1]G. Krausch et al., *Macrocolecules* **33** (3), 947-953, 2000 [2]M. Stamm et al., *JACS* **125** (40), 12211-12216, 2003

CPP 13.28   Tue 14:00   P3

Molecular Dynamics Simulations of Bottle-Brush Co-Polymers with a Rigid Backbone under Poor Solvent Conditions — •PANAGIOTIS E THEODORAKIS, WOLFGANG PAUL, and KURT BINDER — Institute for Physics, Johannes-Gutenberg University, Mainz, Germany

We have performed extensive Molecular Dynamics simulations for a bead-spring off-lattice model of flexible side chains tethered to a rigid backbone under poor solvent conditions. In particular, we study the static conformational properties of bottle-brush macromolecules by varying parameters specific to this molecular architecture, i.e. the grafting density of the side chains and the backbone length. We also compute structure factors describing the scattering from a single side chain and the total bottle-brush polymer. These results are used for the interpretation of experimental scattering data for bottle-brush macromolecules. Furthermore, we examine the structure formation in co-polymer bottle-brushes under marginal to poor solvent conditions for the side chains.

CPP 13.29   Tue 14:00   P3

Structural relaxation process in epoxy nanocomposites as seen by mechanical and dielectric spectroscopy — •MATTHIEU THOMASSEY, JÖRG BALLER, MARKUS ZIEHMER, BARTOSZ ZIELINSKI, MARTINE PHILIPP, ULRICH MÜLLER, JAN KRISTIAN KRÜGER, and ROLAND SANCTUARY — Université du Luxembourg, Laboratory of Physics of Condensed Matter and Advanced Materials (LPM), 162a, avenue de la Faïencerie, L-1511 Luxembourg

Epoxy resins based on diglycidyl ether of bisphenol A (DGEBA) are thermal glass formers with glass transition temperatures of about 250 K. Incorporation of inorganic nanoparticles into these oligomer matrices take influence on their thermal glass transition behaviour. Depending on the interaction between epoxy resin oligomers and nanoparticles the structural relaxation process which is made responsible for the glass transition can be changed. Mechanical and dielectric spectroscopy is used to study the structural relaxation process in two types of nanocomposites: DGEBA filled with silica and alumina nanoparticles. These investigations which are also supported by measurements of the complex specific heat capacity indirectly elucidate the molecular interaction between nanoparticles and oligomer matrix.

CPP 13.30   Tue 14:00   P3

Analysing dielectric interphases in composites containing nano- and micro- particles — •BÉATRICE HALLOUET[1], PAULINE DESCLAUX[1], BERND WETZEL[2], ALOIS SCHLARB[2], and ROLF PELSTER[1] — [1]Universität des Saarlandes, FR 7.2 Experimentalphysik, D-66123 Saarbrücken, Germany — [2]Institut für Verbundswerkstoffe GmbH (IVW), Erwin-Schrödinger-Straße Geb.58, D 67663 Kaiserslautern, Germany

We have investigated a molecular relaxation process in a solid polymer filled with dispersed magnetite particles. Especially, we compare systems containing nano-particles with diameters between 20 and 30 nm and micro-particles with diameters between 0.5 and 5 μm. Temperature-dependent broadband dielectric spectroscopy in a frequency range between 50 Hz and 1 GHz reveals that the presence of nano- or micro-particles does not affect the molecular dynamics. However, there is a marked difference in the polymers relaxation strength reflecting both the polarizability and the number of relaxing units. While in the micro-composites the polymer matrix behaves bulk-like, its relaxation strength increases in the nano-composites, the deviation from the bulk value being proportional to the volume fraction of particles. We discuss the results in terms of interphases of thickness δ around particles and agglomerates, the volume fraction of which increases with increasing particle concentration and decreasing particle size. Additional IR and DSC measurements are used to check whether the chemical properties or the amorphous state of the polymer matrix have been altered by the addition of particles.

CPP 13.31   Tue 14:00   P3

The influence of silica nano fillers on the structure and dynamics of linear polymer melts — KLAUS NUSSER[1,2], •GERALD JOHANNES SCHNEIDER[1,2], WIM PYCKHOUT-HINTZEN[1], LUTZ WILLNER[1], and DIETER RICHTER[1] — [1]IFF, Forschungszentrum Jülich GmbH, Leo-Brandt-Str., 52425 Jülich — [2]Jülich Centre for Neutron Science at FRM2, Lichtenbergstr. 1, 85747 Garching bei München

Elastomer-filler composite materials are technically very important and widely used. In particular, the reinforcing effect achieved by the addition of fillers like silica into a polymer matrix is commonly used to tune macroscopic properties like the elastic modulus of the composite material. In order to get new insight into the microscopic mechanisms of reinforcement, a blend material consisting of a linear polymer (Polyethylene-propylene, polyisoprene and polydimethylsiloxane) and hydrophobized silica was investigated. A study of the rheology of the material in dependence of the filler volume percentage was performed. Moreover Small Angle Neutron Scattering and Neutron Spin Echo experiments were performed in order to get insight into the microscopic structure and dynamics of the systems. In particular, the constraints on the polymer dynamics imposed by the presence of the silica particles were investigated for different filler degrees.

CPP 13.32   Tue 14:00   P3

Nano two-point Microrheology: Structure and Dynamics of Polymer-melts near Tg — •MARKUS SELMKE, SUBHASIS ADHIKARI, and FRANK CICHOS — Molecular Nanophotonics Group, University Leipzig

The structure of glassy polymer melts near their glass transition point has been controversially debated for a long time, and so are the numerous partly successful models suggested for such complex systems. A qualitatively proposed one, the view that cage-like structures form, i.e. soft cavities in-between interlocked stiff polymer-backbone arches, is one among others. To investigate the structure, molecular dynamics in the low M_w glass former glycerol have been studied by Orrit et. al. (2006), and rheological data has been found to agree with SM rotational relaxation times. Our group has not only extended this comparison to the complex high-M_w glass-former PMA, where such a match is far from being evident, but also compared the SM experiments to dielectric data that yields information on local flexibility and reorientation of the matrix the molecules are embedded in, confirming the expected difference in timescales due to different observable physical phenomena underlying the methods (Ngai, 1988). To further study polymer networks, the cross-correlated thermal motion of suitably chosen fluorescent tracer-dyes attached to the ends of bi-functionalized polymer strands is to be explored in the system with FRET on a nm-scale with the method of 2-point microrheology as introduced by (Crocker, 2000). This way, a 1/r-strain-field consistent correlation, or any deviation, is expected to shed light on the cage structure.

CPP 13.33   Tue 14:00   P3

Shapes of two dimensional star polymers — •CHRISTIAN VON FERBER[1,2], YATES MONTEITH[3], and MARVIN BISHOP[3] — [1]Applied Mathematics Research Centre, Coventry University, UK — [2]Physikalisches Institut, Universität Freiburg — [3]Department of Mathematics/Computer Science, Manhattan College, New York, USA

We explore the shapes of excluded volume, two dimensional star polymers by both renormalization group methods and Monte Carlo computer sim- ulation of a tangent hard disk model. The mean-square radius of gy- ration, the g-ratio, and the asphericity of linear and star polymers are examined. The standard expansion for the g-ratio is modified to use the known exact value of the radius of gyration exponent $\nu = 3/4$ rather than only the first order ϵ-expansion value. Good agreement is obtained with the current Monte Carlo Pivot algorithm results and previous simulations of other polymer models. Our approach also improves the predictions of the g-ratio in three dimensions significantly enhancing the accuracy of the renormalization group results for calculating shape properties.

CPP 13.34   Tue 14:00   P3

Characterization of flexible dendrimers by small-angle scattering — •SABINE ROSENFELDT[1], MATTHIAS BALLAUFF[1], and LUDGER HARNAU[2] — [1]Physikalische Chemie I, Universität Bayreuth, Germany — [2]MPI für Metallforschung, Universität Stuttgart, Germany

Solutions of flexible dendrimers are investigated up to volume fractions of 0.23, which is a value slightly over the overlapp concentration of the dendrimers. Small-angle neutron scattering and contrast variation

were used to determine the radial structure and the interparticular interactions. The experimental structure factors will be used to test the valibility of the decoupling approximation of the total scattering intensity. The data were interpretated using the PRISM integral equation formalism. It is shown that the decoupling approach using the form factor of an undisturbed dendrimer is a good approximation, even for the data in the range of the overlapp concentration.