

CPP 8: POSTER: Polymer Physics

Time: Monday 16:00–18:00

Location: Poster B

CPP 8.1 Mon 16:00 Poster B

A Monte Carlo study of a chain in a periodic potential — ●MIRCEA GALICEANU¹, JENS-ÜWE SOMMER², and ALEXANDER BLUMEN¹ — ¹Theoretische Polymerphysik, Universität Freiburg, Hermann-Herder-Straße 3, D-79104 Freiburg, Germany — ²Leibniz-Institut für Polymerforschung Dresden e. V., Hohe Strasse 6, D-01069 Dresden, Germany

We present Monte Carlo simulations of polymer chains of length N in a periodic array of traps. The static quantities, like the effective segment length and the end-to-end distance are controlled by the scaling variable $E = \delta\xi$, where δ is the strength of adsorption and ξ is the distance between two neighboring traps. We study chains with $N = 500$ and 1000 monomers and different values of δ and ξ . That the static quantities depend only on $E = \delta\xi$ is in very good agreement with former results[1]. The dynamic quantities which we study are the mean square displacement of all monomers, the mean square displacement of the center of mass and of the middle monomers relative to the center of mass. Using these results we are able to obtain the relaxation time as a function of the scaling variable E , and can show that at low values of E a chain in a periodic environment obeys a Rouse-like dynamics.

[1] J.-U. Sommer and A. Blumen, *J. Chem. Phys.* **105**, 6008, (1996)

CPP 8.2 Mon 16:00 Poster B

Simulations of Flexible and Semiflexible Polymers: Dynamic and Viscoelastic Properties — ●JULIAN SCHNEIDER^{1,2}, ALEXANDER BLUMEN¹, and MARTIN STEINHAUSER² — ¹Albert-Ludwigs-Universität, Theoretische Polymerphysik, Freiburg — ²Fraunhofer Institut für Kurzzeiddynamik (EMI), Freiburg

Using Molecular-Dynamics-Simulations we investigate the dynamic and viscoelastic properties of single chains and of melt systems consisting of flexible and semiflexible units. In order to find a unified description for such chains we performed simulations with different polymer models and compared the numerical results to standard models. We find good agreement with the scaling-predictions of the Rouse-Model for flexible chains with no significant dependence of the spring-type connecting the beads. For semiflexible chains we observe a $t^{-5/4}$ -decay in the time-dependent shear modulus as recently predicted.

CPP 8.3 Mon 16:00 Poster B

Advanced ultrafast nanocalorimetry: superheating in linear polymers — ●ALEXANDER MINAKOV¹, ANDREAS WURM², and CHRISTOPH SCHICK² — ¹A.M. Prokhorov General Physics Institute, Vavilov 38, 119991 Moscow, Russia — ²University of Rostock, Institute of Physics, Universitätsplatz 3, 18051 Rostock, Germany

To study phase transition kinetics on submillisecond time scale a set of new membrane gauges for ultrafast scanning nanocalorimetry were constructed. Controlled ultrafast cooling, as well as heating, up to 1 million K/s was attained. The dynamic model describing the temperature distribution at ultrafast temperature change in the membrane-gas system was developed. The characteristic rate corresponding to the quasi-static limit of the temperature change in the membrane-gas system was determined. The rate equals 0.1 million K/s for different gauges in helium gas. The method was applied for the measurements of the superheating phenomenon in a set of linear polymers iPS, PBT, PET, iPP. A power law relation between the superheating and the heating rate was observed in the range 0.01 - 10000 K/s of heating rates. A superheating limit about 10% of the melting temperature was found out at the rates above 0.01 - 0.1 millions K/s. This limit depends on the sample crystallization temperature. The observed superheating limit, as well as the power law, can be accounted for the internal stress induced by the superheating near the crystalline-amorphous interfaces in the semicrystalline polymers.

CPP 8.4 Mon 16:00 Poster B

Neue Einsichten in die Strukturbildung von elastomerem Polypropylen — ●MECHTHILD DÖRING, CHRISTIAN DIETZ, SABINE SCHERDEL, NICOLAUS REHSE und ROBERT MAGERLE — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

In unseren Experimenten untersuchen wir dünne Filme von elastomerem Polypropylen (ePP) mit einem sehr niedrigen Polymerisationsgrad. Mit Hilfe des Rasterkraftmikroskops können wir die Kristallisation des zuvor aufgeschmolzenen Materials in situ bei Raumtemperatur

beobachten. Anschließend bilden wir die räumliche Struktur mittels Nanotomographie ab. Auf diese Weise lässt sich der Zusammenhang zwischen dem Prozess der Kristallisation und der räumlichen Struktur der Kristallite besser verstehen. Während der Kristallisation beobachteten wir zahlreiche Phänomene, die sich mit derzeitigen, einfachen Modellen der Strukturbildung nicht vollständig beschreiben lassen, wie zum Beispiel das Aufspalten einer Lamelle. Um diese und andere Beobachtungen näher zu untersuchen, wurde von der Probe mittels Nanotomographie ein Volumenbild des entsprechenden Bereichs erstellt und mit den so erhaltenen Erkenntnissen ein Modell für die jeweiligen Phänomene aufgestellt. Neben dem Effekt der Aufspaltung werden in unserem Beitrag weitere Beobachtungen des Wachstums und der Struktur von ePP-Kristalliten mit den dazugehörigen Modellen vorgestellt und diskutiert.

CPP 8.5 Mon 16:00 Poster B

Dynamik und Struktur von Defekten in dünnen Blockcopolymerfilmen — ●EIKE-CHRISTIAN SPITZNER, MARCUS BÖHME, MARTIN KREIS, CHRISTIAN DIETZ, SABINE SCHERDEL, NICOLAUS REHSE und ROBERT MAGERLE — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

Wir untersuchen Dynamik in Systemen dünner Schichten von Polystyrol-*block*-Polybutadien Copolymeren, die im Volumen hexagonal geordnete Zylinderstrukturen bilden. Die Mikrodomänendynamik der in Chloroformdampf gequollenen Filme verfolgen wir in situ mit Hilfe der Tapping Mode Rasterkraftmikroskopie. Hierbei kommt es zu einer Reihe von charakteristischen Defekten, die teilweise über längere Zeit stabil sind. Beispielsweise sind ringförmige Defekte mit einem Punkt in der Mitte außerordentlich stabil. Ihre Volumenstruktur ist jedoch unbekannt. Die räumliche Abbildung der Defektstrukturen mit der Nanotomographie kann helfen, die Ursachen für ihre Stabilität besser zu erklären. Zudem wird somit auch ein Vergleich mit Ergebnissen aus Simulationen der Strukturbildung ermöglicht.

CPP 8.6 Mon 16:00 Poster B

Nanotomographie an Polypropylen mit hohem Kristallinitätsgrad — ●MARIO ZERSON, MECHTHILD DÖRING, CHRISTIAN DIETZ, NICOLAUS REHSE und ROBERT MAGERLE — Chemische Physik, TU Chemnitz, D-09107

Polypropylen (PP) bildet bei der Kristallisation lamellare Nanostrukturen aus. Die Form, die Ausrichtung und die Konnektivität der Kristallite bestimmen die Eigenschaften des Materials. Für die Charakterisierung der Volumenstruktur verwenden wir die Nanotomographie, die auf der Kombination von Rasterkraftmikroskopie (AFM) und geeigneten Ätzverfahren beruht. Bei dieser Methode wird die Oberfläche wiederholt schrittweise durch ein nasschemisches Ätzverfahren abgetragen und mit dem AFM abgebildet. Auf diese Weise erhält man eine Reihe von Bildern, die die Rekonstruktion der Struktur des PP ermöglicht. Eine Herausforderung stellt dabei der geringe Anteil an amorphen Material dar, der die Zuordnung der individuellen Lamellen nach jedem Ätzschritt erschwert. Wir zeigen unsere aktuellen Ergebnisse zur Nanotomographie an semikristallinen PP. Schwerpunkt der Arbeit ist es das Ätzverfahren zu optimieren, um die räumliche Struktur von PP mit höherem Kristallinitätsgrad abzubilden.

CPP 8.7 Mon 16:00 Poster B

Chemical confinement: Additional modes in the relaxation spectrum of a copolymer — ●JÖRG HACHENBERG¹, BJÖRN STEISEL², DENNIS BEDORF¹, MICHAEL BUBACK², and KONRAD SAMWER¹ — ¹I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — ²Institut für Physikalische Chemie, Universität Göttingen, Tammannstr. 6, 37077 Göttingen, Germany

Copolymers with different monomer distributions but of comparable composition and comparable degree of polymerization have been investigated by mechanical spectroscopy and differential scanning calorimetry. An additional mode occurs in the relaxation spectra of copolymers with a non-random monomer distribution which is absent in those with a random distribution. This is interpreted as the motion of soft block-like segments between rigid segments in the non-random copolymer. These unique features can be found in poly(ethylene-co-methacrylic acid) (EMAA) synthesized by high pressure free radical polymerization

under steady state conditions. Two hydrogen bonds can tighten the methacrylic acid functions forming a chemical confinement in samples with a non-random distribution. The sample properties are controlled by SEC, FTIR and NMR.

This work is supported by DFG, Graduiertenkolleg 782.

CPP 8.8 Mon 16:00 Poster B

Rouse Dynamics in a Random Medium — ●MICHAEL STRAUCH and EKKEHARD STRAUBE — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, D-06099 Halle (Saale), Germany
We have studied the dynamics of a Rouse chain with randomly distributed segmental mobilities and were able to calculate the dynamic structure factor rigorously.

Introducing a *time step* opens up the possibility to extend this model so that the description of the motion of polymer chains inside random media becomes possible. The (randomly distributed) mobilities are no longer constant. Rather, the average mean square displacement (MSD) of the segments between two consecutive time steps is taken as a measure for the mean free path length. After comparing each segment's individual MSD (between consecutive time steps) with this mean free path length a decision is made whether this segment's mobility is altered (because it has moved a sufficient distance within the medium) or not (because it is still in the vicinity of its previous position).

In our poster we present results from our numerical simulations and compare them with experimental data.

CPP 8.9 Mon 16:00 Poster B

Kernspinrelaxationsverhalten und mechanische Eigenschaften von SBS-Blockcopolymeren — ●NIKOLAUS NESTLE, WALTER HECKMANN, KONRAD KNOLL und HELMUT STEININGER — BASF AG Ludwigshafen

SBS-Blockcopolymeren werden bereits seit langem als Mischungskomponente bei der Herstellung schlagzäher und hochtransparenter Styrolkunststoffe eingesetzt. Neben dem Gehalt an Butadienkauschuk sind dabei die Topologie der Ketten und die Verteilung des Butadienanteils über die einzelnen Blöcke des Polymers hinweg entscheidend für die mechanischen Eigenschaften im Gemisch mit reinem Polystyrol. Bei der Analyse von an den reinen Blockcopolymeren gemessenen TD-NMR-Daten und den mechanischen Eigenschaften der mit Polystyrol abgemischten SBS-Materialien zeigen sich deutliche Korrelationen zwischen den Parametern der Magnetisierungsabfallkurven und wichtigen anwendungstechnischen Größen wie z.B. dem E-Modul. Wegen des stärkeren Einflusses unterschiedlicher Mikrophasentopologien sind die keine vergleichbar deutlichen Zusammenhänge zwischen NMR-Größen und mechanischen Eigenschaften bei den reinen SBS-Blockcopolymeren zu beobachten.

CPP 8.10 Mon 16:00 Poster B

Atomic Force Microscopy of Polymer Networks — ●ALEXANDER SCHMATULLA and OTHMAR MARTI — University of Ulm, Institute of Experimental Physics, 89069 Ulm, Germany

We demonstrate the option of a custom built Atomic Force Microscope (AFM) for detection, nanomanipulating and pulling on strains of molecular polymer networks with a resolution on the nanometer scale.

By using contact mode, tapping mode and pulsed force mode we have imaged the polymer network. After detection of the network structure we have moved the AFM tip to a point x/y on the specimen, then we have bent and moved the cantilever in contact well defined distances over the surface. After pulling in contact we have imaged the same area which we have scanned before. The result was that molecular polymer strains of a branched polyethylene have been pulled over well defined distances. In addition we have analyzed the forces while pulling the molecule strains. After pulling the strains we have detected variances not only in the nearer periphery of the pulling area. We will compare our results with other measurement and detection methods (Raman spectroscopy, SEM).

CPP 8.11 Mon 16:00 Poster B

Phase contrast in AFM images of hard-soft polymeric systems — ●ALBRECHT PETZOLD, KLAUS SCHRÖTER, and THOMAS THURN-ALBRECHT — Martin-Luther-University Halle-Wittenberg, Institute of Physics, Experimental Polymer Physics

Tapping mode atomic force microscopy (TMAFM) is widely used to obtain height and phase images of heterogeneous polymeric systems. The influence of sample properties and imaging parameters

on the phase image is still an active area of research. We here present a detailed study about the origin of the phase contrast in polyethylene (PE) as a typical semi-crystalline polymer with a liquid like amorphous phase. The phase signal obtained during imaging of PE is compared to measurements on hard and soft model systems, namely glassy polystyrene (PS) and crosslinked poly(dimethylsiloxane) (PDMS). Force spectroscopy curves of both model polymers were taken to obtain amplitude and phase information depending on the tip-sample distance. The phase signal of PE can be qualitatively understood in comparison to the different phase-distance curves obtained on PS and PDMS. Additionally the influence of several imaging parameters, like excitation frequency, free amplitude and stiffness of the cantilever on the shape of the force spectroscopy curves was investigated. As a result empirical suggestions for imaging of semi-crystalline polymers are made.

CPP 8.12 Mon 16:00 Poster B

Investigation of Internal Energy Change in Strain Experiments — ●SUSANNA HERZOG, GERALD JOHANNES SCHNEIDER, and DIETMAR GÖRITZ — Institut für Physik, Universität Regensburg, 93040 Regensburg

Due to the deformation of an elastomer the deformation energy and the heat energy change. One fundamental assumption of polymer physics is the total conversion of both energies, which implies no change of the internal energy by the first law of thermodynamics. There is however a change of the internal energy in deformation experiments. A possible explanation for this effect is the modification of the sample's volume.

In our measurement we can determine the amount of the internal energy by measuring the expended work and heat for the deformation.

CPP 8.13 Mon 16:00 Poster B

Diblock copolymer systems with boundaries and electric fields — ●MARIANNE BREUER and BARBARA DROSSEL — Institut für Festkörperphysik, Technische Universität Darmstadt, Deutschland

Block copolymer melts are a good model system for the study of molecular self-assembly. We investigate the nature, stability and dynamics of formation of diblock copolymer structures under different boundary conditions. We examine the effects of strong electric fields. We employ both numerical and approximate analytical treatments which are based on mean-field theory of the standard Gaussian model.

CPP 8.14 Mon 16:00 Poster B

Surface characterization of electron-beam irradiated polymer brushes — ●SINA BURKERT, FRANK SIMON, CORNELIA BELLMANN, PETRA UHLMANN, and MANFRED STAMM — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, D-01069 Dresden, Germany

Polymer brushes out of PS, P2VP, PNIPAM and PAA were used to modify and control the surface potential of Si-wafers. The polymers brushes formed layers of thickness of less than 20 nm and significantly changed the surface potential of the substrate, which was investigated with contact angle measurements. Their chemical composition was studied by XPS. Electron irradiation was employed to modify the brushes by different radiation doses. With XPS and Zeta-potential measurements we were able to specify the surface composition after electron beam treatment. Changes in surface composition and the structure of the grafted polymer brushes allowed to qualify cross-linkages and degradation processes. By varying the dose we could adjust on the one hand the decomposition of the polymer and on the other hand the amount of hydrophilic groups. We know that the adsorption of proteins on polymers highly depends on the surface potential. This work could be used to control the surface potential of the polymer brush as well as the adsorption of proteins, only by varying the radiation dose. The chosen substrate silicon is also attractive for lab-on-chip applications of those modified brushes.

CPP 8.15 Mon 16:00 Poster B

Adiabatic crystallization of polycaprolactone — ●ANDREAS WURM¹, YUJI MIYAZAKI², KUMIKO MIWA², AKIRA INABA², and CHRISTOPH SCHICK² — ¹University of Rostock, Institute of Physics, Polymerphysics, 18051 Rostock, Germany — ²The Research Center for Molecular Thermodynamics, Graduate School of Science, Osaka University TOYONAKA, OSAKA 560 0043 JAPAN

Existence and formation of pre-ordered structures as the initial step of polymer crystallization are discussed controversially. Most of the findings and interpretations are based on scattering experiments, which test small density differences between the assumed precursors of the

crystals and the surrounding melt. Because of the low contrast the interpretation of experimental results becomes often speculative. Contrary relaxation experiments are probing motions in the sample and are therefore independent on density contrast. During crystallization material is transformed from the liquid to the solid state. Consequently, motions (fluctuations) typical for a liquid become impossible and do not longer contribute to the measured relaxing signal. For pre-ordered structures we expect some changes in mobility too because of the changes in conformation on pre-ordering. Adiabatic calorimetry is suitable to detect temperature changes in the sample, which can be related to crystallinities below one thousandth. In this study we compare crystallinity data from adiabatic calorimetry in the sub-percent range with complex dielectric permittivity of ϵ -polycaprolactone (PCL) during isothermal crystallization.

CPP 8.16 Mon 16:00 Poster B

Monte Carlo Simulations for Associate Formation in Semi-Dilute Polymer Solutions — ●MARIAN BRANDAU, STEFFEN TRIMPER, and EKKEHARD STRAUBE — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale)

The results of a lattice-free dynamic Monte Carlo simulation for a semi-dilute polymer rod-bead system are presented.

We assume that the associate formation is determined by a small number of attractive saturable groups. Furthermore, the reactive monomers are supposed to be distributed randomly over the chains and are able to react mutually.

Starting from a dense well equilibrated melt configuration we extract a certain amount of chains, again randomly, which are subjected to the dynamic simulation according to a Metropolis algorithm.

The quantity of interest is the time evolution of the cluster structure depending on the chain density, the density of the reactive groups and the reaction rate. In particular, we find a cluster distribution function.

CPP 8.17 Mon 16:00 Poster B

Fluctuation Effects in the Theory of Microphase Separation in Diblock Copolymers in the Presence of an Electric Field — ●ILJA GUNKEL, SEMJON STEPANOW, THOMAS THURN-ALBRECHT, and STEFFEN TRIMPER — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle

We generalize the Fredrickson-Helfand theory of the microphase separation in symmetric diblock copolymer melts by taking into account the influence of a time-independent homogeneous electric field on the composition fluctuations within the self-consistent Hartree approximation. We predict that electric fields suppress composition fluctuations, and consequently weaken the first-order transition. In the presence of an electric field the critical temperature of the order-disorder transition is shifted towards its mean-field value.

We also compute the collective structure factor in the disordered phase, which becomes anisotropic in the presence of the electric field. Fluctuational modulations of the order parameter along the field direction are suppressed. The latter correlates with the parallel orientation of the lamellae in the ordered state.

CPP 8.18 Mon 16:00 Poster B

Texture control in PVDF nanotubes — ●NITIN SHINGNE^{1,2}, MARKUS GEUSS², LILI ZHAO², MARTIN STEINHART², ULRICH GÖSELE², ELKE HEMPEL¹, and THOMAS THURN-ALBRECHT¹ — ¹Department of Physics, Martin Luther University, D-06120, Halle — ²Max-Planck-Institute of Microstructure Physics, D-06120, Halle

Using DSC and WAXS we studied the crystallization of poly(vinylidene fluoride) nanotubes templated inside the pores of ordered porous alumina. The crystal texture resulting from isothermal crystallization strongly depends on the crystallization temperature. We observed that crystallization at lower temperatures led to statistical orientation of the crystallites modified by growth under the conditions of 2D confinement. However, at high crystallization temperatures the 1D nanostructures shows a uniform crystal orientation with the (020)-direction pointing along the pore axes. Crystallization has to be initiated independently in each of the separated nanotubes, most likely by homogeneous nucleation. We assume that the orientation observed at low crystallization temperature reflects the random orientation of the nuclei and additionally a selection of growth direction along the pore axes, whereas at high crystallization temperatures the growth along different crystal directions seems to be highly selective leading to the well defined crystal orientation within the nanotubes. Therefore, by choosing the crystallization temperature, control of crystal orientation within the 1D nanostructures is possible. This approach could pave the

way for the reversible adjustment of ferro- and piezoelectric properties of the 1D polymeric nanostructures.

CPP 8.19 Mon 16:00 Poster B

Phase behaviour and transition of polymer-brushes on Microcantilevers — ●SEBASTIAN LENZ and JOCHEN GUTMANN — Max Planck Institute for Polymeric Research, Mainz

Polymer brush coatings are well known for their ability to tailor surface properties in a wide range of applications. In most cases, brushes are used in solution. Here we show that the micromechanical cantilever (MC) sensor technique is a tool to perform time-resolved physico-chemical investigations of the phase behaviour and phase transition of thin polymeric layers. Complementary to scattering techniques for measuring the thickness, MC sensor technique provides information about changes in the internal pressure of brushes during a phase-transition.

CPP 8.20 Mon 16:00 Poster B

Combined AC and fast scanning chip calorimetry — ●HEIKO HUTH, ALEXANDER MINAKOV, and CHRISTOPH SCHICK — Universität Rostock, Institute für Physik, Universitätsplatz 3 18051 Rostock

In the recent years new calorimetric techniques were developed using chip calorimeter based on thin film and silicon technology. Using these chips it is possible to reach fast heating and cooling rates up to 100.000 K/s. This gives new insight in the kinetic of polymer crystallization and reorganization processes not available with standard DSC devices. Another possibility is an extreme sensitive AC calorimetry for very small samples. Due to the fact of the small addenda heat capacity the measured sample is also in the range of nanogram. Here it is possible to measure thin polymer films below 10 nm. The next task was the combination of the advantage of both methods. Using the AC method the investigation of slow processes is possible with high sensitivity. Using fast scanning calorimetry the preparation of the sample prior to the measurement as avoiding crystallization is possible. This gives access to the crystallization kinetics from glass transition to melt for most of the semi crystalline polymers. First investigations of crystallization kinetics with the combined method on different semi crystalline polymers are presented.

CPP 8.21 Mon 16:00 Poster B

Distribution function of a wormlike chain with a fixed orientation of — ●SEMJON STEPANOW and FEDOR SEMERIYANOV — Universität Halle, Institut für Physik, 06099 Halle

We study the distribution function of the three dimensional wormlike chain with a fixed orientation of one chain end using the exact representation of the distribution function in terms of the Green's function of the quantum rigid rotator in a homogeneous external field. The transverse 1d distribution function of the free chain end displays a bimodal shape in the intermediate range of the chain lengths ($L_p, \dots, 3.5 L_p$). We present also analytical results for short and long chains, which are in complete agreement with the results of previous studies obtained using different methods.

CPP 8.22 Mon 16:00 Poster B

Thermomechanical Investigations of Filled Rubbers — ●WILLIBALD HENGL, GERALD JOHANNES SCHNEIDER, and DIETMAR GÖRITZ — Institut für Physik, Universität Regensburg, 93040 Regensburg

The reinforcing mechanism of rubber fillers is still an interesting topic. We made investigations of uniaxial elongation of filled rubbers by deformation calorimetry, whereby the change of internal energy can be calculated from the measured mechanical work and heat.

We present experiments mainly on silica-filled Polydimethylsiloxane (PDMS) with varying filler content and silica with and without a silane additive. As filled elastomers usually show strain-softening, the extensions have been repeated.

Although there are different stress-strain relations for each experiment, it is found, that the change of internal energy is predominantly controlled by the true stress acting on the specimen, independent of the composition and the history of the samples.

CPP 8.23 Mon 16:00 Poster B

In-situ-Beobachtung und statistische Auswertung der Strukturbildung in dünnen Blockcopolymer-Filmen — ●MARCUS BÖHME, SABINE SCHERDEL, NICOLAUS REHSE und ROBERT MAGERLE — Chemische Physik, TU Chemnitz, D - 09107 Chemnitz

Wir untersuchen mittels Tapping Mode Rasterkraftmikroskopie *in situ* die Strukturbildung in dünnen Filmen eines zylinderbildenden Polystyrol-*block*-Polybutadien-Blockcopolymeren in einer definierten Chloroformdampf-Atmosphäre. Dabei beobachten wir die Entstehung und Ausheilung von Einzeldefekten sowie Reorientierungen vorgeordneter Strukturen in der Nähe struktureller Phasenübergänge, deren Lage im Phasendiagramm durch den Lösungsmittelgehalt und die Dicke des Filmes bestimmt werden. Die statistische Auswertung zeigt enge zeitliche Zusammenhänge zwischen den beobachteten Erscheinungen und Änderungen im Lösungsmittelgehalt des flüssigen Filmes.

CPP 8.24 Mon 16:00 Poster B

Pulling on Single Siloxane Molecules — ●PETER SCHWADERER¹, CHRISTOPH BRÄUCHLE¹, ENNO FUNK², FRANK ACHENBACH², JOHANN WEIS³, and JENS MICHAELIS¹ — ¹Department Chemie und Biochemie, Ludwig-Maximilians-Universität München, Butenandtstraße 5-13, D-81377 München — ²Wacker Chemie AG, Johannes-Hess-Strasse 24, D-84489 Burghausen — ³Consortium für elektrochemische Industrie GmbH, Zielstattstr. 20, D-81379 München

Siliconelastomers are high-performance materials, used in a wide field of applications. Among their remarkable qualities are low temperature dependence of the mechanoelastic properties, high resilience against thermooxidation, high flexibility at low temperatures, inadhensive behavior and physiological harmlessness. On the other hand siliconelastomers also have some disadvantages like low ultimate mechanical strength, vulnerability to hydrolytic reagents and moisture expansion in unipolar environment. Single molecule force spectroscopy using an AFM offers a unique possibility to investigate the mechanical performance of single siloxane polymer chains and their fixation in thin polymer networks. Both theoretical as well as experimental single molecule measurements can help to gain insights into the properties of the Si-O bond.

CPP 8.25 Mon 16:00 Poster B

Temperature Dependence of the Payne Effect — ●ANDREAS MICHAEL SCHMIDT¹, ANTJE BERGMANN², GERALD JOHANNES SCHNEIDER¹, and DIETMAR GÖRITZ¹ — ¹Institut für Physik, Universität Regensburg, 93040 Regensburg — ²Institut für Theoretische Festkörperphysik, Abteilung für Didaktik der Physik, Universität Karlsruhe, 76128 Karlsruhe

The "Payne-Effect" is an interesting phenomenon which can be observed in filled elastomers. It is characterised by a decline in the dynamical shear modulus with increasing deformation.

Instead of performing a conventional shear experiment we measured the shear force using a needle that could penetrate the sample periodically.

With our experimental setup we are able to vary the penetration depth, the deformation amplitude and the frequency of the needle oscillation.

We investigated SBR systems filled with VN3 silica, in which the filler content was varied. Furthermore, we performed annealing treatments on the samples and studied the filler rearrangement in the rubber matrix.

CPP 8.26 Mon 16:00 Poster B

Temperature resolved investigation of grating formation on azobenzene polymer films. — ●PADMANABH VEER¹, ULLRICH PIETSCH¹, and PAUL ROCHON² — ¹Dept. of Solid State Physics, University of Siegen, ENC, Siegen, 57068, Germany. — ²Dept. of Physics, Royal Military College, Kingston, Ontario, Canada, k7l3ng.

It was discovered 10 years ago that the exposure of an initially flat surface layer of an azobenzene-containing polymer to a holographic light pattern leads to the formation of surface relief structures (SRG) accompanied by a mass transfer over several micrometer. Many authors have investigated the process of SRG formation [1,2]. However, the nature of the driving force of this process is still unclear. We performed temperature resolved inspections of the SRG formation. The experiment was performed in a vacuum chamber to avoid the hot air turbulence. The sample is illuminated with circularly polarised light of wavelength 514nm and probed with He-Ne laser of wavelength 633nm. Inspecting the first order diffraction peak of a He-Ne laser, it has been seen that the grating inscription rate as well as the grating efficiency decrease with increasing sample temperature. No SRG formation is possible approaching the glass transition temperature 'T_g' of the polymer film. A simple model considering two competitive processes can explain the data, the light induced alignment of chromophores along the valleys of the SRG and the thermally induced disorder of chromophores. [1]

Rochon, P. et. al. Appl. Phys. Lett. 1998,72,2096. [2] Barrett, C. et. al. J. Phys. Chem. 1996,100,8836

CPP 8.27 Mon 16:00 Poster B

Crystallization behavior of pure iPS and iPS filled with nanoparticles — ●MOHAMED ISMAIL, ANDREAS WURM, and CHRISTOPH SCHICK — University of Rostock, Inst. of Physics, Polymerphysics,

In this contribution we demonstrate the crystallization behavior of pure iPS and iPS filled with nanoparticles by using DSC instrument. - We measured the heat capacity of pure iPS samples and iPS nanocomposites - The samples were prepared with different contributions of nanoparticles by solving iPS in a toluol and addition the nanoparticles as well as applied the ultra sonic on the samples to distribute the nanoparticles through the polymer matrix. Finally, we dried the samples. - From the heat capacity data we obtained informations about the crystalline fraction, C, the rigid amorphous fraction, RAF, and the mobile amorphous fraction.

CPP 8.28 Mon 16:00 Poster B

The effect of matrix molecular weight on the interfacial morphology of iPP fiber/matrix single polymer composites — ●XIAOLI SUN, HUIHUI LI, and SHOUKE YAN — State Key Laboratory of Polymer Physics and Chemistry, Institute of Chemistry, The Chinese Academy of Sciences, Beijing 100080, P.R. China

To prepare samples of β -iPP, selective β -nucleants are commonly used. Moreover, crystallization of commercial iPP in temperature gradient, and forcing shearing in melt can also encourage the development of the β -phase.

In our previous studies, the interfacial structure of the iPP fiber/matrix polymer composites as a function of the fiber introduction temperature, fiber molecular weight as well as the subsequent crystallization temperature of the matrix was studied. It was found that partial melting of the iPP fiber is in favor of the formation of β -iPP crystals. In the present study, the influence of matrix molecular weight on the induced interfacial structure was studied. The matrix with lower molecular weight can be easily initiated to form β -iPP cylindrite by incomplete molten iPP fiber as researched previous. The matrix with higher molecular weight, however, cannot be induced to form β -iPP cylindrite when the isothermal crystallization is equal to 135 °C. But when using β -nucleating agent this matrix is able to effectively form β -spherulites when the isothermal temperature is under 140 °C. This can be explained in terms of different requirement for different matrix molecular weight chain to form β -iPP when iPP fiber was used to induce its matrix crystallization.

CPP 8.29 Mon 16:00 Poster B

Nanocalorimetric study of syndiotactic poly(propylene) (sPP) with different content of carbon nanotubes — ●SERGEY ADAMOVSKY¹, FELICE DE SANTIS², and CHRISTOPH SCHICK¹ — ¹Institute of Physics, University of Rostock, Universitaetsplatz 3, 18051 Rostock, Germany — ²Department of Chemical and Food Engineering, University of Salerno, 84084 Fisciano (SA), Italy

Polymer carbon nanotube composites attracted a great deal of attention in recent years. It is known, that electrical conductivity, shear viscosity, other mechanical and thermal properties of polymers are strongly influenced by the presence of small amounts (fractions of percent) of carbon nanotubes (CNT). Crystallization behaviour as well as crystal structure should be affected too.

A novel technique [1], based on a nanocalorimetric chip [2] was applied to study the crystallization of syndiotactic poly(propylene) (sPP) filled with different amount of carbon nanotubes. A pure sPP was measured as a reference. Sample mass of as small as about 100 ng allows us to use a heating/cooling rates of up to 500000 K/s which extends the rate range available in DSC dramatically. Together with DSC a range of cooling rates of 0.005 K/s to 500000 K/s was covered. A strong dependence of the crystallization temperature on cooling as well as of the crystallization half-time during isothermal crystallization on the CNT-content was observed.

1. S Adamovsky, C Schick. *Thermochimica Acta*, Vol. 415, Issue 1 (2004) Pages 1-7.

2. Xensor Integration, www.xensor.nl

CPP 8.30 Mon 16:00 Poster B

Rheo-FTIR studies on spider silk — ●JAN SÖLTER, PERIKLIS PADOPOULOS, and FRIEDRICH KREMER — Institut für Experimentelle Physik I, Universität Leipzig, Linnéstr. 5, 04103, Leipzig

Spider silk has unique mechanical properties which are currently not met by man-made materials. To study the interrelationship between (microscopic) molecular structure and the (macroscopic) mechanical response a polarized time-resolved FTIR-spectrometer is combined with a custom-made setup to measure the complex mechanical modulus. For that a dense wire grid of single parallel arranged spider threads of *Araneus diadematus* is prepared and a step-like increase of the strain is applied while measuring the resulting stress. The specificity of the IR spectral range enables one to trace in detail the microscopic response of the different molecular moieties, i.e. the reorientation and the order parameter, the phase relation within the molecular system with respect to the mechanical excitations and possible memory effects.

CPP 8.31 Mon 16:00 Poster B

Isothermal crystallization of PVDF using ultra-fast nano-calorimetry — ●EVGENY ZHURAVLEV¹, ARKADIUSZ GRADYS², ALEXANDER MINAKOV^{1,3}, and CHRISTOPH SCHICK¹ — ¹Institute of Physics, University of Rostock, Germany — ²Institute of Fundamental Technological Research, Polish Academy of Sciences, Warsaw, Poland — ³General Physics Institute, Moscow, Russia

By means of ultra fast thin-film nano-calorimetry, we were able to perform non-isothermal crystallization of poly(vinylidene fluoride) at cooling rates up to 10000 K/s. The new technique allows us to study samples of about 12 ng mass. Sample mass was estimated from measured heat capacity. At rates 12000 K/s and higher we were able to produce amorphous PVDF. At successive heating we observe so called cold crystallization. Isothermal crystallization of PVDF was investigated. Crystallization kinetics was studied at millisecond time scale. Experiments were performed from melt and from amorphous state of PVDF.

CPP 8.32 Mon 16:00 Poster B

Analysis of the microdomain dynamics in thin films of block copolymers — ●SABINE SCHERDEL¹, KLAUS MECKE², CHRISTIAN FRANKE¹, MARCUS BÖHME¹, and ROBERT MAGERLE¹ — ¹Chemische Physik, TU Chemnitz, D-09107 Chemnitz — ²Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, D-91058 Erlangen

We investigate the structure formation in thin films of polystyrene-*block*-polybutadiene copolymers. With modern atomic force microscopes we record series of images with high temporal and spatial resolution in a relatively short time. The manual analysis of these data, however, takes often months. To accelerate the quantitative analysis we use and compare different image processing methods. By computing local Minkowski measures we get important morphological information about the geometry of the observed structures and their evolution with time. Another way to characterize structures is to reduce them to their medial axis and to identify and count the branching points of the skeletonized structure. Their temporal evolution and characteristic time constants are analyzed with correlation functions.

CPP 8.33 Mon 16:00 Poster B

Development of Entanglements in a Polymer Melt — ●THOMAS VETTOREL, THOMAS A. VILGIS, and KURT KREMER — Max-Planck-Institut fuer Polymerforschung, 55128 Mainz, Germany

Recent work by Rastogi et al. has shown that it is possible to prepare a polymer melt in an initially disentangled state. This system then relaxes to the normal, entangled melt state but gives rise to a long-lived metastable "new melt" in which different parts of the chains exhibit different mobilities due to an unusual distribution of entanglements. This yields a material whose particular mechanical properties could be of interest for many purposes.

We study the mechanisms leading to the relaxation to the entangled state by means of computer simulations, using a normal bead-spring model, with and without explicit bending rigidity. A fully disentangled polymeric system is created as a collection of chains collapsed in a globular state, packed together at the melt density. We then monitor the relaxation of this strongly out-of-equilibrium system, looking more particularly at the evolution of the entanglements: The entanglement length N_e is measured using the Primitive Path Analysis.

The first results show that in the case of relatively short chains (up to $N \approx 20N_e$), the relaxation of the entanglement length is very fast, suggesting that the situation is better described by a scenario like de Gennes' explosion upon melting, even if a slowing down is observed in the diffusion of chains' centers of mass before equilibrium is reached, indicating a confinement effect.

CPP 8.34 Mon 16:00 Poster B

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CPP 8.35 Mon 16:00 Poster B

Surface functionalization by ultrathin plasma polymer coatings: From partial coverage to closed films — JAKOB BARZ^{1,2}, MICHAEL HAUPT¹, CHRISTIAN OEHR¹, and ●ACHIM LUNK² — ¹Fraunhofer IGB, Nobelstr. 12, 70569 Stuttgart — ²Institut für Plasmaforschung, Universität Stuttgart, Pfaffenwaldring 31, 70569 Stuttgart

Plasma processes based on different monomer precursors are successfully applied to deposit ultrathin polymer films onto different substrate materials. The film thickness and the chemical composition of the polymer are greatly influenced by the choice of the precursor, the deposition time, the electric power, the pressure, and additional gases.

In order to study various deposits, plasma processes were performed in a trifluoromethane (CHF_3) discharge, diluted by argon.

By the variation of the above parameters, the coating thickness varied between 0.5 and 10 nm as determined by spectroscopic ellipsometry. The surface tension was determined according to the Owens-Wendt-Rabel-method; for coatings above 2.9 nm thickness, the surface energy remained constant, independent from the polymer thickness or the discharge parameters, at values of 15 mN/m disperse and 0.2 mN/m polar surface tension. At lower thicknesses, differences between advancing contact angles (representing the low-energy parts) and receding contact angles (representing high energy surface contributions) were observed. In the examined coatings, this behavior is attributed to the partial inset of polymer growth for mild plasma conditions, and further correlated to data from AFM and XPS measurements.

CPP 8.36 Mon 16:00 Poster B

Photovoltaic Devices Based on Semiconducting Block-Copolymers — ●S HUETTNER¹, S LINDNER², A CHICHE¹, G KRAUSCH¹, and M THELAKKAT² — ¹Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth, Germany — ²Makromolekulare Chemie I, Universität Bayreuth, 95440 Bayreuth, Germany

We investigate the concept of photovoltaic devices based on block copolymers. The use of a functionalized block copolymer made of electron donor (D) and acceptor (A) polymers lead to a self assembled microstructure that insures the photon to be absorbed within a very short distance (tens nm) to the D-A interface. A block copolymer made of a poly(vinyltriphenylamine) (D) and poly(perylene bisimide acrylate) (A) has been synthesized [1]. Photovoltaic devices made of such a copolymer film have shown significantly better efficiencies than similar devices made from a blend of the corresponding homopolymers [2]. The reason for that clearly lies in the different morphologies. The blend-based device exhibits a phase separation resulting in micron sized domains and resulting in an important loss of post-absorption excited states that cannot reach the interface.

[1] S. Lindner, M. Thelakkat, *Macromolecules* 37, 8832 (2004) [2] S. Lindner, S. Hüttner, A. Chiche, M. Thelakkat, G. Krausch, *Angew. Chem. Int. Ed.* 45, 3364 (2006)

CPP 8.37 Mon 16:00 Poster B

Self assembly of a crystalline block copolymer in a selec-

tive solvent — ●A.M. MIHUT¹, A. CHICHE¹, H SCHMALZ², and G KRAUSCH¹ — ¹Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth, Germany — ²Makromolekulare Chemie I, Universität Bayreuth, 95440 Bayreuth, Germany

We investigate the formation and growth of complex supramolecular structures formed by a crystalline diblock copolymer (PEO-PB) in a selective solvent. The interaction between the crystalline block and

the solvent can be controlled by the temperature. While cooling the system, the solvent (heptane) becomes a selective solvent for the amorphous block (PB). The resulting structure is related to the interplay between the phase separation and the crystallization of the PEO block. We study the effects of the experimental conditions (cooling rate and final temperature) as well as the molecular parameters on the morphology of the supramolecular objects by scattering techniques and electron microscopy.