CPP 32: Polymer Physics III

Time: Thursday 9:30–12:00 Location: ZEU 222

CPP 32.1 Thu 9:30 ZEU 222

Bulk Behaviour of Random Block Copolymers — •Birger Steinmüller and Marcus Müller — Institut für Theoretische Physik, Georg-August-Universität Göttingen

The microphase separation of random block copolymers is a promising route for fabricating fuel cell membranes. In order to describe this process on time and length scales, which are not accessible by atomistic simulations, we resort to coarse-grained models. We use a coarse-grained bead-spring model in conjunction with MD simulations and study a soft-particle model by Single-Chain-in-Mean-Field (SCMF) simulations. The advantages of the MD model are its operation with a model of higher resolution than SCMF, therefore it can be better mapped to results of atomistic simulations, and that it permits a more immediate access to dynamical quantities of polymer melts and solutions. The SCMF model on the other hand is a simpler one, which employs softer interactions and is thus computationally far more efficient. We want to propose a strategy for mapping the SCMF to the MD model. Thus, we will be able to benefit from the advantages of both models.

We discuss our results with a focus on the methodology used to parametrize the SCMF model with the aim of reproducing the mesoscale behaviour of the MD model. The approach is validated by comparing structural properties of the models on said scale.

CPP 32.2 Thu 9:45 ZEU 222

Modelling of hysteresis behaviour of multigraft copolymers — •Ralf Schlegel[1], Daniel Wilkin[1], Ulrike Staudinger[1,5], Roland Weidisch[1], Jimmy W. Mays[2], David Uhrig[3], and Nikos Hadjichristidis[4] — [1]Institute of Materials Science and Technology (IMT), Friedrich-Schiller-University Jena, Löbdergraben 32, D-07743 Jena, Germany — [2]Department of Chemistry, University of Tennessee, Knoxville, USA — [3]Center for Nanophase Materials Science at ORNL, PO BOX 2008 MS6494, Knoxville, TN USA — [4]Department of Chemistry, University of Athens, Athens 15771 Greece — [5]current address: Institute of Materials Science, Technische Universität Dresden, 01062 Dresden, Germany

Multigraft copolymers are thermoplastic elastomers with a special molecular architecture. Polystyrene(PS) arms are grafted regularly spaced and with different functionalities onto a rubbery polyisoprene(PI) backbone chain. Graft functionality and the number of grafting points can be controlled at synthesis level. The hysteresis properties of multigraft copolymers have been critically investigated. TEM investigations revealed that the materials are showing micro phase separation. The non-affine tube model of Kaliske and Heinrich was applied and adapted to the stress release curve of the materials. In addition to the model parameters a parameter describing the stress softening is attained. Multigraft copolymers with tetra and hexafunctional molecular architecture were characterized. Significant low stress softening characteristics were observed for the tetrafunctional materials with spherical PS micro domains.

CPP 32.3 Thu 10:00 ZEU 222

Traveling spatially periodic forcing of phase separation — •Vanessa Weith, Alexei Krekhov, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany

Within the framework of a suitably generalized Cahn-Hilliard model [1,2] we present a theoretical analysis of phase separation of binary polymer mixtures in the presence of spatially periodic forcing of wavenumber q traveling with a velocity v.

We found that for a stationary forcing ($v = 0$) phase separation is locked beyond a critical forcing amplitude $a_0(q)$ to periodic patterns of wavenumber $Q = q$. This critical amplitude is increased at increasing the pulling velocity v. The bifurcation diagram, the existence range of the periodic solutions, as well as the dynamics of phase separation influenced by the forcing have been studied.

We have also investigated the existence and stability of subharmonic periodic patterns of wavenumber $Q = q/m$ ($m \geq 2$) and their spatio-temporal behaviour for the cases $v = 0$ and $v \neq 0$. We obtained that the critical forcing amplitudes for the stabilization of subharmonic periodic patterns are larger than for the harmonic solution with $Q = q$.

[1] A. P. Krekhov and L. Kramer, Phys. Rev. E **70**, 061801 (2004)

[2] V. Weith, A. Krekhov and W. Zimmermann, Eur. Phys. J. B, in press (2008)

CPP 32.4 Thu 10:15 ZEU 222

Modelling agglomeration effects in CNT/polymer composites — •Marina Saphiannikova, Sven Richter, and Gert Heinrich — Leibniz-Institute für Polymerforschung, Hohe str. 6, 01069 Dresden

Theoretical description of viscoelastic properties of the polymer melts, filled with attractively interacting anisometric particles, represents a great challenge. Such filler particles tend to build a network-like superstructure [1] which is very fragile and can be easily broken in external flow fields. In the quiescent state the particles agglomerate again, slowly restoring the network superstructure. In this study, to describe the agglomeration/deagglomeration process of anisometric particles, we use a superposition approach, in which the total stress is represented by a sum of three stresses: 1) the viscoelastic stress arising in the polymer matrix, 2) the hydrodynamic reinforcement due to the presence of anisometric particles, 3) the viscoelastic stress arising in the filler network. The latter is represented by a nonlinear variant of the Maxwell model combined with a usual kinetic equation for the scalar structural parameter that describes the instantaneous state of filler network at particular flow conditions. This approach is verified in a number of linear and nonlinear shear experiments carried out on polycarbonate composites filled with carbon nanotubes [2].

This work was supported by the BMBF grant CarboNet No.03X0504E.

[1] F.R.Costa et al. Adv. Polym. Sci. 210, 101 (2008) [2] S.Richter et al. Submitted to Macromol. Symp., Macromolecules

CPP 32.5 Thu 10:30 ZEU 222

Anisotropy of the dynamic mechanical properties of strongly stretched polymer networks — •Vladimir Toshchevikov[1,2], Gert Heinrich[1], and Yuli Gotlib[2] — [1]Leibniz Institut für Polymerforschung, Dresden, Germany — [2]Institute of Macromolecular Compounds, Saint-Petersburg, Russia

Superposition of large static and small oscillating strains has been proposed recently as a method for studying the structure of polymer networks [1,2]. The main goal of the present work is to study the anisotropy of the dynamic mechanical properties of strongly stretched polymer networks with respect to the direction of a static strain. This is of importance to understand the crack propagation in rubbers, which is determined by the dynamics of highly stretched network portions near crack tips under pulsed loading conditions (http://www.ipfdd.de/FOR597). We show that a stretched polymer network is characterized by the anisotropy of viscoelastic properties: frequency dependent shear modulus is different for different geometries of applying the shear (parallel or perpendicular to the axis of deformation). For all geometries of the shear, fine structure of the relaxation spectrum leads to the broadening of the frequency dependences of loss moduli which can display several maxima at strong deformations. Theoretically calculated frequency dependences of the loss and storage moduli are in a good agreement with experimental data [2].

This work was supported by the RFBR (08-03-00150).

[1] V.L.Bodneva et al. Polymer Science 2005, 47, 409

[2] E.Munch et al. Polymer 2006, 47, 3477

15 min. break

CPP 32.6 Thu 11:00 ZEU 222

Combination of μGISAXS and imaging ellipsometry - a new versatile instrument for the surface sensitive investigation of polymer films — •Volker Körstgens[1], Robert Meier[1], Johannes Wiedersich[1], Stephan V. Roth[2] und Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department LS E13, James-Franck-Str. 1, D-85747 Garching — [2]HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg

For the structural investigation of polymer thin films the method μGISAXS (grazing incidence small angle x-ray scattering with a μm-sized beam) is well established and very powerful. It gives access to lateral structures at the surface as well as buried structures of inhomogeneous samples such as gradient films. Whereas in the common setup available at a few beamlines at synchrotron radiation sources the

samples are investigated with μGISAXS and simultaneously with optical microscopy, we introduce an advanced method with in-situ imaging ellipsometry replacing the optical microscopy. Therewith a comprehensive sample characterization is possible including local film thickness and optical properties combined with structural information with a spatial resolution depending on the size of the x-ray beam. The scope of the instrument is illustrated with investigations on different polymer samples. Full capability of the method will be reached with implementation in the newly developed μSAXS/WAXS beamline at the novel high-brilliance synchrotron radiation source PETRA3 at DESY, Hamburg beginning its operation in fall 2009.

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CPP 32.7 Thu 11:15 ZEU 222

Investigating industrial processes at the future microSAXS/WAXS beamline at PETRA III — •Stephan V. Roth, Adeline Buffet, Ralph Döhrmann, Hermann Franz, Rainer Gehrke, Heinz Graafsma, Patrick Grögor, Ulrich Ulrich Hahn, Michael Lohmann, Ralf Röhlsberger, Horst Schulte-Schrepping, and Edgar Weckert — HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany

Micro- and nanofocused x-ray beams combined with small- and wide-angle x-ray scattering (SAXS/WAXS) are powerful tools to investigate nanocomposite and hierarchical materials on multiple length scales. In 2009, the microfocusSAXS/WAXS beamline P03 will become operational at PETRA III. This beamline combines high resolution in both real and reciprocal space with beam sizes ranging from 40μm to 100nm. The low divergence offered by the high-β-undulator allows for installing ultraSAXS geometries in combination with such small beams. We present the detailed layout of the μSAXS/WAXS beamline. Strong emphasis is put on the future improvements of the various experimental IN-SITU scanning techniques, such as nano- and microbeam GISAXS [1,2] and micro/nanoSAXS tomography [3] as well as its possible combinations with high-througput and industrial processing methods for thin film technology and fluidics.

[1] S.V. Roth et al., Appl. Phys. Lett 91, 091915 (2007)
[2] E. Metwalli et al., Langmuir 24, 4265 (2008)
[3] C. Schroer et al., Appl. Phys. Lett. 88, 164102 (2006)

CPP 32.8 Thu 11:30 ZEU 222

Recent Experiments at the SAXS Beamline BW4 — •Andreas Timmann, Ralph Döhrmann, Tom Schubert, Stephan V. Roth, and Rainer Gehrke — HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg, Germany

The BW4 beamline at HASYLAB is a versatile small-angle x-ray scattering (SAXS) beamline. It offers transmission and grazing incidence SAXS using sample-detector distances (D_{SD}) between one meter and 13 meters. For $D_{SD} < 2$m it also offers a moderate micro-focus of $22 \times 40\mu m^2$ at sample position. All SAXS techniques can be combined with wide-angle x-ray scattering.[1]

Recently we conducted in-situ GISAXS experiments such as rheology and sputter-deposition.[2,3]

We also examined a beryllium compound refractive lens (Be-CRL) as focusing optic for USAXS geometries. Its usage results in an undistorted beam and the background is considerable lower than that caused by focusing mirrors[4]

References:

[1] Roth et al., Rev. Sci. Instrum., 2006, 77, 085106
[2] Timmann et al., App. Phys. Let., 2007, 91, 213102
[3] E. Metwalli et al., Langmuir, 2008, 24, 4265
[4] Timmann et al., Rev. Sci. Instrum., submitted

CPP 32.9 Thu 11:45 ZEU 222

High Intensity - High Resolution Small-Angle Neutron Diffractometers of JCNS at FRM II — •Aurel Radulescu — Jülich Centre for Neutron Science (JCNS), Forschungszentrum Jülich GmbH, 85747 Garching, Deutschland

The KWS-1 and KWS-2 small-angle neutron diffractometers of Jülich Centre for Neutron Science are currently reconstructed at the Research Neutron Source Heinz Maier-Leibnitz (FRM II) in Garching-München. With a high flux supplied by the cold neutron source of FRM II and the newly designed optimized neutron guide and with a new collimation system allowing a larger experimental flexibility the instruments will be dedicated facilities for structural studies in the field of soft-matter and magnetic systems. The standard of 5x5 cm2 neutron guides leads to high intensities with standard resolution and provides a maximum flux close to world leading SANS instruments, as for example D22, ILL-Grenoble. Further support is obtained by neutron lenses that allow for larger sample apertures of 5x5 cm2 without loosing any resolution. High counting rates (up to 600kHz) will be detectable with a dead-time of about 0.6 microsec for either homogeneous or strong inhomogeneous scattering patterns distributed on the scintillation detector. The high resolution mode is supported by a chopper, which will allow a variation of the wavelength spread between 10% (as delivered by the velocity selector) and 1%. Additionally, the neutron lenses in combination with small collimation apertures lead to smallest Q-vectors of around 0.0001 1/Å. The high intensity and high resolution options of the KWS-1 and KWS-2 SANS instruments will be presented in details.