

CPP 19: Focus: Soft Matter and Nanocomposites - New opportunities with advanced neutron sources II

Time: Monday 15:00–17:00

Location: ZEU 222

CPP 19.1 Mon 15:00 ZEU 222

TOF-NR investigation of cononsolvency in PNIPAM-based block copolymer thin films — ●CHRISTINA GEIGER¹, LUCAS P. KREUZER¹, TOBIAS WIDMANN¹, PEIXI WANG¹, ROBERT CUBITT², CRISTIANE HENSCHL³, ANDRÉ LASCHEWSKY³, CHRISTINE M. PAPADAKIS⁴, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — ²Institut Laue-Langevin, 38042 Grenoble, France — ³Fraunhofer-Institut für Angewandte Polymerforschung, 14476 Potsdam, Germany — ⁴TU München, Physik-Department, Physik weicher Materie, 85748 Garching, Germany

The diblock copolymer PMMA-*b*-PNIPAM forms micelles in aqueous solution that exhibit a reversible shell collapse transition at the lower critical solution temperature (LCST). Apart from a temperature stimulus, the collapse can also be induced upon addition of organic cosolvents due to the competitive attachment and detachment of water and cosolvent to the PNIPAM chains. We demonstrate that the cononsolvency effect is transferrable from solutions to thin polymer films. The film swelling and collapse kinetics due to the uptake of water and cosolvent from a saturated vapor atmosphere are investigated with a focus on time-of-flight neutron reflectometry (TOF-NR). Sequential contrasting experiments using protonated and deuterated compounds are performed to differentiate between the distributions of water and cosolvent within the polymer films.

CPP 19.2 Mon 15:15 ZEU 222

On the structure and inner dynamics of zwitterionic polysulfobetaine brushes — ●JUDITH WITTE¹, OLAF HOLDERER², JÖRG LAHANN^{3,4}, and STEFAN WELLERT¹ — ¹Technische Universität Berlin, Berlin, Germany — ²Heinz Maier-Leibnitz Zentrum, Garching, Germany — ³University of Michigan, Ann Arbor, MI, USA — ⁴Karlsruhe Institute of Technology, Karlsruhe, Germany

PMEDSAH brushes are zwitterionic polysulfobetaine brushes, which are investigated as a microenvironment for the attachment and lift-off of cells and proteins. Structure and dynamics of polymer brushes influence the motion of macromolecules, nanoparticles or proteins at and along the interface and their potential adsorption at or penetration into the brushes. So far, a rather simple approach is used to discuss the complex self-association behavior. Still, a more detailed understanding of the structure and dynamics within PMEDSAH brushes, especially of the self-association behavior, is lacking. We conduct a series of complementary laboratory and neutron scattering experiments to improve the basic understanding of the influence of the grafting density on the brush structure and inner dynamics. Beside X-ray-reflectometry and ellipsometry measurements on dry polysulfobetaine brushes with different grafting densities also multi contrast neutron reflectometry measurements on the wet brushes were performed to investigate the brush structure in dependence on the grafting density. Additionally, neutron spin echo spectroscopy under grazing incidence is applied to study the influence of the self-association on the segmental dynamics in the polysulfobetaine brushes.

CPP 19.3 Mon 15:30 ZEU 222

Structural characterization and rheology of biocompatible wormlike micelles - comparing experiment and theory — ●BENJAMIN VON LOSPICHL^{1,2}, SABINE H. L. KLAPP², and MICHAEL GRADZIELSKI¹ — ¹Institut für Chemie, Technische Universität Berlin, Straße des 17. Juni 124, D-10623 Berlin — ²Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin

Wormlike micelles exhibit a unique viscoelastic behaviour, which has been investigated intensely in the past decades by experimentalists and theoreticians [1,2]. Within our studies we explore the self-assembled structures and the flow behaviour of biocompatible wormlike micelles, which are a mixture of a short-chained C₈ cationic surfactant and the salts of long-chained C₁₈ to C₂₂ omega-9 fatty acids. The variation of the omega-9 fatty acids yields a change in thickness of the micelles, which strongly influences the flowing properties of the system. To characterize the size distribution and the relaxation time of the micellar solutions we use neutron scattering, rheology and electric birefringence. The obtained experimental results are then quantitatively compared

to an established theoretical model describing the dynamics of micelles under shear. The model links mechanical properties such as stress to structural quantities like alignment or micellar length [3].

[1] C. Dreiss, *Soft Matter* **3**, 956, (2007)[2] P. D. Olmsted, *Rheo. Acta* **47**, 283, (2008)[3] B. v. Lospichl, S. H. L. Klapp, *Phys. Rev. E* **98**, 042605, (2018)

CPP 19.4 Mon 15:45 ZEU 222

Polyelectrolyte Multilayer Films from Mixtures of Polyanions: Different Composition in Film and Preparation Solution — ●ANNEKATRIN SILL, ANTONIA WELTMAYER, PETER NESTLER, MALTE PASSVOGEL, SVEN NEUBER, and CHRISTIANE A. HELM — University Greifswald, Institute of Physics, Germany

Polyelectrolyte multilayer films were prepared from polyanion PSS and polycation PDADMA in 0.1 M NaCl by sequential adsorption of oppositely charged polyelectrolytes. PSS consisted of binary mixtures of long deuterated PSSd (Mw(PSSd) = 80.8 kDa) and short protonated PSS (Mw(PSS) = 10.6 kDa). With neutron reflectivity, it was found that the mole fraction of long PSSd in the film exceeded the one in the deposition solution. Indeed, the film consisted of only PSSd if the mole fraction of PSSd in the deposition solution exceeded 5%. This observation can be explained by the adsorption kinetics which were studied with in-situ ellipsometry. Two mechanisms determined the film composition: (i) during PSS deposition, adsorption of short PSS was reversible while adsorption of long PSSd was irreversible; thus, the PSSd fraction increased with adsorption time; (ii) if short PSS was present, each polycation adsorption step was followed by slow desorption of polyelectrolyte complexes consisting of PDADMA and short PSS molecules. Short PSS is bound with fewer electrostatic monomer/monomer bonds to the film and can easier desorb, or form complexes with PDADMA. These studies show how to measure and control film composition when polydisperse polyelectrolyte solutions are used for film preparation.

CPP 19.5 Mon 16:00 ZEU 222

Functional Nanocomposites: Neutron Scattering Study — ●MARGARITA KRUTEVA¹, LISA FRUHNER^{1,2}, ARTUR FELD³, RIEKE KOLL³, HAUKE HELLER³, JÜRGEN ALLGAIER¹, WIM PYCKHAUT-HINTZEN¹, ARTEM FEOKTYSTOV⁴, OLAF HOLDERER⁴, MICHAELA ZAMPONI⁴, HORST WELLER³, and STEPHAN FÖRSTER¹ — ¹Jülich Centre for Neutron Science (JCNS-1) and Institute for Complex Systems (ICS-1), Forschungszentrum Jülich GmbH, Germany — ²Institute of Physical Chemistry, RWTH Aachen University, Aachen, Germany — ³Institut für Physikalische Chemie, Universität Hamburg, Germany — ⁴Jülich Centre for Neutron Science JCNS at MLZ, Garching, Germany

Nowadays adaptive synthetic polymer materials which are able to change their properties on demand play important role in nanotechnology. In contrary to conventional polymer nanocomposites, the nanoparticles functionalized with a polymeric shell, which takes the role of a matrix, allow to control the distance between the nanoparticles and homogeneously dispersed per definition. Determining factors are size of the core, grafting density, length of the grafting chain and temperature. Supramolecular functionalization (H-bonds) of the grafting chains leads to additional steps in adaptiveness. Moreover, using magnetic nanoparticle as a core extends the application area to e.g. magnetorheological nanocomposites. In this talk I will focus (1) on the structure of magneto-elastomeric nanocomposites with supramolecular activity and (2) polymer chain dynamics in one component nanocomposites (OCNC) studied by neutron scattering.

CPP 19.6 Mon 16:15 ZEU 222

Morphology investigation of the active layer of hybrid solar cells with TOF-GISANS — ●VOLKER KÖRSTGENS¹, LAUTARO DIAZ PIOLA¹, CHRISTINA GEIGER¹, JULIAN HEGER¹, LUCAS KREUZER¹, ANNA-LENA OECHSLE¹, TOBIAS WIDMANN¹, MATTHIAS NUBER², KLARA STALLHOFER², GAETANO MANGIAPIA³, HRISTO IGLEV², REINHARD KIENBERGER², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — ²TU München, Physik Department, LS Laser- und Röntgenphysik, James-Franck-Str. 1, 85748

Garching — ³Helmholtz-Zentrum Geesthacht am Heinz Maier-Leibnitz Zentrum, Lichtenbergstr. 1, 85747 Garching

One aspect for the development of non-conventional solar cells should be the sustainability of the production process of devices. Following this idea, we developed hybrid solar cells which can be processed out of aqueous solution. The active layer of these devices is based on laser-processed titania nanoparticles dispersed in a water-soluble polythiophene. The active layers were produced with two of the most common deposition techniques: spray deposition and slot die coating. With these techniques the thickness of layers can be easily controlled and the scale-up toward the coating of large areas is done with low effort. We investigated the morphology of the deposited active layers with time of flight - grazing incidence small angle neutron scattering (TOF-GISANS). The difference of the morphology of these layers is presented and its impact on the performance of devices is discussed.

CPP 19.7 Mon 16:30 ZEU 222

Ionic liquid cation dynamics in carbon nanoconfinement: A pore size and temperature-dependent neutron spectroscopy study — ●MARK BUSCH¹, TOMMY HOFMANN², BERNHARD FRICK³, JAN P. EMBS⁴, BORIS DYATKIN⁵, and PATRICK HUBER¹ — ¹Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — ²Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — ³Institut Laue-Langevin, Grenoble, France — ⁴Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, Villigen, Switzerland — ⁵Dept. of Materials Science and Engineering, Drexel University, Philadelphia, U.S.A.

The temperature-dependent cation dynamics of the room-temperature ionic liquid [BuPy][Tf₂N] within the nanoconfinement of carbide-derived carbons with various pore sizes are investigated by quasi-elastic neutron spectroscopy. An overview of the dynamic landscape over a wide temperature range is obtained by employing fixed window scans, where one sample parameter is scanned, while only one specific energy transfer value is observed. These data that provide already a quite

comprehensive understanding of the confinement-induced alteration of the molecular mobility in comparison to the bulk are complemented by a more detailed analysis of full energy transfer spectra. Two diffusive processes on different time scales are found. Both are considerably slower than in the bulk and the corresponding self-diffusion coefficients decrease with decreasing nanopore size. In spite of this dynamic slow down, the temperature range of the liquid state upon nanoconfinement is found to be notably extended to much lower temperatures.

CPP 19.8 Mon 16:45 ZEU 222

The impact of water on functional nanocellulose thin films — ●CALVIN J. BRETT^{1,2}, LUCAS P. KREUZER³, TOBIAS WIDMANN³, ELISABETTA NOCERINO¹, OLA K. FORSLUND¹, LIONEL PORCAR⁴, PETER MÜLLER-BUSCHBAUM^{3,5}, MARTIN MÅNSSON¹, DANIEL L. SÖDERBERG¹, and STEPHAN V. ROTH^{1,2} — ¹KTH Royal Institute of Technology, Stockholm, Sweden — ²Deutsches Elektronen-Synchrotron, Hamburg, German — ³Technische Universität München, Lehrstuhl für Funktionelle Materialien, Garching, Germany — ⁴Institut Laue-Langevin, Grenoble, France — ⁵Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany

Sustainable devices experience a massive increase of attention over the last decade. Our whole economy is starting to minimize the use of fossil resources. Nevertheless, it is yet not fully understood how sustainable devices perform and degrade under environmental influences and how we could improve possible drawbacks. Cellulose, as one of the most earth abundant nature materials, consists of so-called cellulose nanofibrils. These nanoscale building blocks have high potential in applications due to their low density, high material strength and sustainability. Within this project, we show how to manufacture materials with desired physical properties such as electrical conductance, optical transmittance, and the tunability of wetting behavior. For real-life applications, we tested the water impact on these functional thin films by applying humidity and studying the films by means of grazing incidence small-angle neutron/X-ray scattering (GISAXS/GISANS) at P03 / PETRA III (Hamburg) and D22 / ILL (Grenoble).