

CPP 10: INTERNAL SYMPOSIUM Scattering Experiments I

Time: Tuesday 9:30–12:30

Location: H37

Invited Talk

CPP 10.1 Tue 9:30 H37

Polymer dynamics: From Synthetic Polymers to Biopolymers — •DIETER RICHTER — Forschungszentrum Jülich, Institut für Festkörperforschung, 52425 Jülich, Germany

In polymeric materials the structures, the macroscopic mechanical and rheological properties and the phase changes are determined to high degree by thermal motion of the atoms and molecules. Most of the relevant dynamics takes place on mesoscopic lengths and time scales in between the picosecond atomic scale and the macroscopic frame. Offering the proper space time observation window, neutron spin echo (NSE) spectroscopy uniquely addresses these motions. We briefly present some key experimental results on the mesoscopic dynamics of polymer systems. We address briefly the standard model of polymer motion, the Rouse model, the role of topological confinement as expressed in the reptation model and finally, processes limiting the confinement * we discuss contour length fluctuations and constraint release of entangled chains. Very recently it became also possible to directly identify large scale internal dynamics of proteins by neutron spin echo. We report the results of these pioneering studies, which most likely will initiate further experiments on the large scale motions of proteins and their relation to the function.

CPP 10.2 Tue 10:00 H37

Glass-Forming Microemulsions and Liquid Dynamics in Soft Confinement — •THOMAS BLOCHOWICZ¹, TINKA SPEHR¹, ANNIKA FRICKE¹, MARTIN MÜLLER¹, BERNHARD FRICK², and BERND STÜHN¹ — ¹TU-Darmstadt, Germany — ²ILL, Grenoble, France

Recently glass forming liquids have been investigated subject to nanoscale geometrical confinements of various kinds, in order to access changes in the molecular dynamics when the confinement comes close to a characteristic lengthscale of cooperative motion. Most experiments were performed with glass formers confined in nanopores in case of which, however, actual finite size effects are superposed with pressure effects or interactions with the confining walls. A different situation can be found in microemulsions, where, droplets of a hydrophilic substance are stabilized by surfactant molecules in a hydrophobic environment. When the substances involved are chosen properly vitrification in a so-called "soft confinement" can be observed. In our particular case we study droplets of glycerol in a matrix of toluene and m-xylene stabilized by the ionic surfactant AOT. The temperature dependent structure of these systems is investigated by small-angle X-ray and neutron scattering, whereas for the dynamical behaviour quasielastic neutron scattering techniques are particularly useful due to their nanoscale spatial resolution. We present time-of-flight and backscattering measurements to access the dynamics of glycerol inside the emulsion droplets. As compared to bulk glycerol pronounced acceleration of the dynamics is observed whereas comparison of core and shell dynamics of the micelles yields almost identical behaviour.

CPP 10.3 Tue 10:15 H37

Starlike dendrimers in solutions: Structural properties and internal dynamics — •SILKE RATHGEBER¹, MICHAEL MOKENBUSCH², JAMES L. HEDRICK³, MIKAEL TROLLSAS³, and ALICE P. GAST⁴ — ¹Max-Planck Institut für Polymerforschung, Polymer Physik, D-55128 Mainz, Germany — ²Forschungszentrum Jülich GmbH, Institut für Festkörperforschung, D-52425 Jülich, Germany — ³IBM Almaden Research Center, San Jose, California 95120-609, USA — ⁴Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 0213, USA

We measured the shape and the internal dynamics of starlike dendrimers under good solvent conditions with small-angle neutron scattering and neutron spin-echo spectroscopy, respectively. [1] Architectural parameters such as the spacer length and generation were varied in a systematic manner. Structural changes occurring in the dendrimers as a function of these parameters are discussed. A first cumulant evaluation of the NSE spectra for each scattering vector q separately yields the length scale dependent relaxation rates $\Omega(q)$. We observe a local minimum in the normalized relaxation rates $\Omega(q)/q^3$ on length scales corresponding to the overall dendrimer dimension. The dynamics is discussed within a Rouse-Zimm approach generalized to the case of starlike dendrimers of arbitrary geometry. The model allows an identification of the modes contributing to the relaxation of the

dendrimer. The local minimum is due to collective breathing motions of (parts of) the dendrons relative to each other. Shape fluctuations are not observed. [1] S. Rathgeber et. al., J. Chem. Phys. **125**, 204908 (2006)

CPP 10.4 Tue 10:30 H37

Neutron Spectroscopy on nono-confined polymers in comparison with dielectric and thermal results — •ANDREAS SCHOENHALS¹, BERNHARD FRICK², MARIA MAYOROVA³, and REINER ZORN³ — ¹Federal Institute of Materials Research and Testing, Unter den Eichen 87, D-12205 Berlin — ²Institut Laue-Langevin, B.P. 156, F-38042 Grenoble — ³Research Center Jülich, Institute for Solid State Research, D-52425 Jülich

The effect of a nanometre confinement on matter is an interesting problem of soft-matter physics. Neutron scattering (NS) is valuable tool to investigate such systems because of the high penetration depth of neutrons. Incoherent NS was carried out on poly(dimethyl siloxane) and poly(methyl phenyl siloxane) confined to Sol/Gel-glasses (7.5, 5.0, 2.5 nm). To cover a broad dynamical range of the scattering function $S(Q,E)$ time-of-flight and backscattering are combined. For the Boson peak the vibrations at lowest frequencies are depressed by the confinement. The mean square displacement msd was calculated from elastic scans. Above T_g the characteristic increase of the msd found for the bulk is strongly influenced by the confinement but for both materials in a different manner. The main influence of the confinement on $S(Q,t)=FT(S(Q,E))$ is a broadening of $S(Q,t)$ with increasing confinement. These results are discussed together with dielectric measurements. This comparison gives strong evidence that (1) the thermodynamic state in a nanometer confinement is different from that of the bulk and that (2) an inherent length scale might exist for the glass transition.

CPP 10.5 Tue 10:45 H37

The boson peak: Theory of scattering from vibrational excitations in disordered materials — •WALTER SCHIRMACHER¹, BERNHARD SCHMID¹, GIANCARLO RUOCCO², and TULLIO SCOPIGNO² — ¹Physik-Dept. E13, TUMünchen, D-85747 Garching — ²Dipt. di Fisica, Univ. di Roma, I-00185 Roma

A theory of vibrational excitations in disordered materials¹ and their observation by inelastic light, neutron, X-ray² and nuclear γ -ray scattering³, based on a model with fluctuating shear moduli is presented. The enhancement of the vibrational density of states (DOS) $g(\omega)$ over Debye's $g(\omega) \propto \omega^2$ law ("boson peak") is shown to be a direct consequence of the disorder. The observed spectra in coherent scattering experiments do not in general reveal the DOS directly. Only in incoherent neutron experiments and in nuclear resonant scattering of synchrotron radiation the scattering law is proportional to $g(\omega)$. Raman spectra are shown to reveal the imaginary part $\Sigma''(\omega)$ of the disorder-induced self energy, which is only indirectly related to the DOS, namely to its enhancement over the Debye DOS. The high-frequency sound damping, observed as broadening of the Brillouin line, is also proportional to $\Sigma''(\omega)$. It is shown that the existing spectra can be consistently interpreted in the light of this theory.

[1] W. Schirmacher, Europhys. Lett. **73**, 892 (2006)

[2] W. Schirmacher, G. Ruocco, T. Scopigno, submitted to Phys. Rev. Lett.

[3] A. I. Chumakov *et al.* Phys. Rev. Lett. **92**, 245508 (2004)**15 min. break****Invited Talk**

CPP 10.6 Tue 11:15 H37

Time-resolved small-angle neutron scattering — •ROLAND MAY — Institut Max von Laue - Paul Langevin, BP 156, F-38042 Grenoble Cedex 9, France

Small-angle neutron scattering has a history of about 40 years, but only with the advent of modern fast electronics has it become feasible to penetrate into time regimes that are compatible with reaction rates and process times of biomolecules, polymers and colloids at full detector resolution. Neutron sources cannot compete with the flux or brilliance of X-ray sources. Therefore they are limited as far as the observation of very fast processes is concerned, unless if they can

be easily and often repeated, as in cyclic events. Of course, neutrons have the special advantage of neutron contrast variation, allowing one to highlight parts of a structure, and they do not produce any radiation damage. This contribution will address these technical issues and give a number of examples from the slow kinetics of oil droplet formation to the observation of the photocycle of photo-active yellow protein in the tens of milliseconds range, and also mention how one can reach even shorter times with sophisticated time-of-flight techniques.

CPP 10.7 Tue 11:45 H37

Protein Interactions in Aqueous Solution Studied by Small-Angle X-ray Scattering — ●FAJUN ZHANG¹, MAXIMILIAN SKODA^{1,2}, ROBERT JACOBS³, RICHARD MARTIN⁴, CHRISTOPHER MARTIN⁵, and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — ²PTCL, University of Oxford, UK — ³CRL, University of Oxford, UK — ⁴Department of Physics, University of Bath, UK — ⁵SRS, Daresbury, Warrington, UK

We have studied protein interactions in two related systems by small-angle x-ray scattering: a series of pure protein solutions with various salt and protein concentrations, and mixtures of protein with oligo(ethylene glycol) (OEG) thiol decorated gold colloids. Structure factors derived from hard sphere potential, screened Coulomb potential, and square well potential, combined with an oblate ellipsoid form factor are used to fit the scattering intensities. An interaction phase diagram has been constructed as a function of ionic strength and protein concentration [1]. For the mixture of protein with functional gold colloid, we present evidence for an attractive interaction between OEG-decorated gold colloids and a repulsive interaction between gold colloid and protein. The attractive potential originates from a depletion force which strongly depends on the size of colloids and the concentration of protein, while the repulsive potential is due to the protein resistance of the OEG monolayer. Indeed, we observed the aggregation of gold colloids, when protein concentration is higher than a critical value.

[1] Zhang, F.; Skoda, M.W.A.; Jacobs, R.M.J.; Martin, R.A.; Martin, C.M.; Schreiber, F. *J. Phys. Chem. B* 2006, in press.

CPP 10.8 Tue 12:00 H37

Surfactant Phase Transitions: New Insights From Time-resolved Small-angle Scattering Experiments — ANNIINA SALONEN¹, JACQUES LENG², PETER SCHURTENBERGER³, and ●STEFAN EGELHAAF⁴ — ¹Institute of Chemistry, Karl Franzens University, 8010 Graz, Austria — ²LOF unité mixte CNRS/Rhodia/Bordeaux, 33608 Pessac, France — ³Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland — ⁴Condensed Matter Physics Labora-

tory, Heinrich-Heine-University, 40225 Düsseldorf, Germany

Most early studies on surfactant systems have addressed their equilibrium behaviour. These remain a prerequisite for further progress, but attention is turning to nonequilibrium phenomena. I plan to present two recent projects in this area:

First, time-resolved small-angle neutron scattering is used to investigate the intermediate structures during the growth of mixed micelles. The growth of the micelles is induced by a reduction in total surfactant concentration, which is realized by rapid mixing of a surfactant solution with buffer. The subsequent structural changes are followed by time-resolved small-angle neutron scattering.

Second, structural changes during the dissolution of lamellar phase are studied with small-angle x-ray scattering. After contact with water, lamellar phase can form fascinating interface instabilities, so-called myelins. Using time and space resolved small-angle x-ray scattering we investigate the changes in the lamellar phase during the formation and growth of these structures.

CPP 10.9 Tue 12:15 H37

Mapping the local nanostructure inside a specimen by tomographic small-angle x-ray scattering — ●JAN M. FELDKAMP¹, CHRISTIAN G. SCHROER¹, MARION KUHLMANN², STEPHAN V. ROTH², RAINER GEHRKE², NORBERT STRIBECK³, ARMANDO ALMENDAREZ-CAMARILLO³, and BRUNO LENGELER⁴ — ¹Institute for Structural Physics, Dresden University, D-01062 Dresden, Germany — ²HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany — ³Institute of Technical and Molecular Chemistry, Hamburg University, Bundesstrasse 45, D-20146 Hamburg, Germany — ⁴II. Physikalisches Institut, Aachen University, D-52056 Aachen, Germany

Small-angle x-ray scattering is combined with scanning microtomography to reconstruct the small-angle diffraction pattern in the direction of the tomographic rotation axis at each location on a virtual section through a specimen. These data yield information about the volume-resolved local nanoscale structure of the sample. With rotational symmetry present in the diffraction patterns, e.g., for isotropic or fiber-textured local nanostructure, the full reciprocal space information in the small-angle scattering regime can be reconstructed at each location inside the specimen. The resolution in real space is determined by the size of the x-ray beam. The experiments were performed with the microbeam option at HASYLAB beamline BW4.

Using this new method, we prove the existence of a skin-core structure in injection molded samples, which cannot be detected in classical tomography.