

CPP 33: Focus Session: Soft Matter and Nanocomposites: New Opportunities with Advanced Neutron Sources 1

organized by Stephan Förster (FZ Jülich), Thomas Gutberlet (FZ Jülich), Peter Müller-Buschbaum (TUM) and Walter Richtering (RWTH Aachen)

Time: Thursday 9:30–11:15

Location: H38

Invited Talk

CPP 33.1 Thu 9:30 H38
Cooperative and non-Gaussian dynamics of entanglement strands in polymer melts — ●MARGARITA KRUTEVA¹, MICHAELA ZAMPONI², INGO HOFFMANN³, JÜRGEN ALLGAIER¹, LUTZ WILLNER¹, ANDREAS WISCHNEWSKI¹, MICHAEL MONKENBUSCH¹, and DIETER RICHTER¹ — ¹Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-1: Neutron Scattering and Biological Matter), 52425 Jülich, Germany — ²Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ, Lichtenbergstraße 1, 85748 Garching, Germany — ³Institut Laue-Langevin (ILL), B.P. 156, F-38042 Grenoble Cedex 9, France

We report neutron spin echo investigations on the motion of short tracer chains in highly entangled melts [1,2]. The tracers were found to undergo sub-diffusion behavior. Unexpectedly the sub-diffusion is limited by a distance very close to the tube diameter of the respective highly entangled host. The cross-over distance to Fickian diffusion, thereby, is independent of the tracer's length. The Fickian diffusivity agreed with the macroscopic results. We found that the Rouse dynamics of the tracers is strongly non-Gaussian with a related segment displacement distribution narrower than the Gaussian counterpart. These results were understood as a consequence of highly cooperative motion of the tracers with the host that mirrors the host dynamics within the tube. The phenomena were found both in a polyolefin (polyethylene) as well as in a polyether (polyethylene-oxide) indicating their generality. (1) Zamponi, M. et al. Phys. Rev. Lett. 2021, 126 (18), 187801. (2) Kruteva, M. et al. Macromolecules 2021, accepted.

CPP 33.2 Thu 10:00 H38
Molecular weight dependent dynamics of polymers grafted on nanoparticles. — ●AAKASH SHARMA¹, MARGARITA KRUTEVA¹, MICHAELA ZAMPONI², SASCHA EHLERT¹, DIETER RICHTER¹, and STEPHAN FÖRSTER¹ — ¹Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-1: Neutron Scattering and Biological Matter), 52425 Jülich, Germany — ²Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ, Lichtenbergstraße 1, 85748 Garching, Germany

Grafting polymer chains on nanoparticles prevents their undesired aggregation leading to improved properties. Whereas, grafting induces inevitable alteration in the dynamics of polymer chains, which affects macroscopic properties e.g. viscoelasticity. It has been established that the polymer chain dynamics is retarded in grafted chains. However, literature lacks consensus on whether the segmental dynamics of grafted chains is accelerated or retarded. We study the segmental dynamics of polyisoprene grafted on spherical nanoparticles using neutron backscattering. The analysis of relaxation times led to the conclusions: (i) Low molecular weight (MW) grafted polymer display reduced local relaxation (ii) At high MW and equal grafting density faster segmental dynamics than the free polymer is observed. We prove that these conflicting results are seemingly artifacts of the traditional analysis method. We invoke an elegant methodology and show that the underlying physics of grafted polymer is unchanged. However, spatial variation of the relaxation times across the grafted chain causes the average dynamics to transition with molecular weight.

CPP 33.3 Thu 10:15 H38
Structure and Dynamics of Polymer Brushes and Microgels at Interfaces measured with Neutron Scattering — ●OLAF HOLDERER¹ and STEFAN WELLERT² — ¹Jülich Centre for Neutron Science at MLZ, Forschungszentrum Jülich GmbH, 85748 Garching, Germany — ²Department of Chemistry, Technische Universität Berlin, 10623 Berlin, Germany

It is an experimental challenge to access structural and dynamic properties of brushes and microgels at the solid liquid interface [1]. Neutron scattering techniques such as Grazing Incidence Small Angle Neutron Scattering (GISANS) for structural investigations and Grazing Incidence Neutron Spin Echo Spectroscopy (GINSES) provide a means of studying structural and dynamic properties on molecular length scales at the interface. Simulations of the experimental conditions in

the framework of the Distorted Wave Born Approximation help interpreting the static and dynamic scattering signals [2]. Examples of thermoresponsive microgels with different architecture and brushes at the interface are presented to illustrate the possibilities and challenges of this type of interface studies.

[1] J. Witte, T. Kyrey, J. Lurtzki, A.M. Dahl, M. Kühnhammer, R. von Klitzing, O. Holderer, S. Wellert, ACS Appl. Polym. Mater. 2021, 3, 2, 976-985

[2] T. Kyrey, M. Kaneva, J. Witte, R. von Klitzing, S. Wellert, O. Holderer, J. Appl. Cryst. (2021) 54, 72-79

CPP 33.4 Thu 10:30 H38
In-situ neutron reflectometry measurements of polyelectrolyte diffusion in Layer-by-Layer films in aqueous solution at ILL — ●ANNEKATRIN SILL¹, HEIKO AHRENS¹, OLAF SOLTWEDEL², PHILIPP GUTFREUND³, and CHRISTIANE A. HELM¹ — ¹University of Greifswald, Institute of Physics, D-17489 Greifswald, Germany — ²Technische Universität Darmstadt, Institute for Condensed Matter Physics, D-64289 Darmstadt, Germany — ³Institut Laue-Langevin, F-38042 Grenoble, France

Up to now, we measured vertical polyelectrolyte diffusion in Layer-by-Layer films by immersing the film for a defined amount of time in the annealing solution. Then the film was dried, and a snapshot was taken. With the snapshot method, one can get good results, but we wanted to develop an improved method. For the first time, the dynamics of our films were studied in-situ at the Institut Laue-Langevin (ILL) on instrument D17. This neutron reflectometer with horizontal scattering geometry is suitable for in-situ measurements, using wavelengths from 2 to 27 Å with great flexibility in resolution. We used the slab architecture with selective polyanion deuteration to study vertical polyanion diffusion. As polycation linear PDADMA was used, PSS/PSSd was the polyanion. Each film consisted of a protonated and a deuterated slab. Varied were the salt concentration and the temperature of the annealing solution. The diffusion constant was determined and compared to the snapshot measurements in air.

CPP 33.5 Thu 10:45 H38
Kinetics of mesoglobule formation and dissolution in solutions of thermoresponsive polymers after fast pressure jumps — BART-JAN NIEBUUR¹, LEONARDO CHIAPPISI², ALFONS SCHULTE³, and ●CHRISTINE M. PAPADAKIS¹ — ¹Technical University of Munich, Physics Department, Garching, Germany — ²Institut Laue-Langevin, Grenoble, France — ³University of Central Florida, Department of Physics and College of Optics and Photonics, Orlando FL, U.S.A.

The thermoresponsive polymer poly(*N*-isopropylacrylamide) (PNIPAM) features lower critical solution temperature behavior in aqueous solution with the cloud point depending on pressure [1]. Fast pressure jumps across the coexistence line in combination with time-resolved small-angle neutron scattering elucidate the pathways of mesoglobule formation and disintegration over a wide range of length scales with a time resolution of 50 milliseconds. Varying the start and target pressures gives insight into the role of thermodynamic and kinetic factors governing mesoglobule formation [2,3]. For disintegration, the osmotic pressure of the solvent within the mesoglobules is the decisive factor for the mechanism and the time scales [4]. These results are of importance for applications of thermoresponsive polymers as switches. 1. B.-J. Niebuur et al., ACS Macro Lett. 6, 1180 (2017). 2. B.-J. Niebuur et al., ACS Macro Lett. 7, 1155 (2018). 3. B.-J. Niebuur et al., Macromolecules 52, 6416 (2019). 4. B.-J. Niebuur et al., RSC Nanoscale 13, 13421 (2021).

CPP 33.6 Thu 11:00 H38
Simultaneous SAXS/SANS method: A novel nanoanalytical tool — ●EZZELDIN METWALLI¹, KLAUS GÖTZ¹, TOBIAS ZECH¹, CHRISTIAN BÄR¹, ANNE MARTEL², LIONEL PORCAR², and TOBIAS UNRUH¹ — ¹Institute for Crystallography and Structural Physics (ICSP), Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 3, 91058 Erlangen, Germany — ²Institut Laue-Langevin, 71, Av-

enue des Martyrs, Grenoble, 38042, France

Exploiting X-ray and neutron beams at the same sample volume enables unprecedented investigations of nanomaterials using small angle scattering (SAS) technique. A portable small angle X-ray scattering (SAXS) instrument with a proper geometrical dimension was successfully designed, constructed and implemented at D22 zone of Institut Laue Langevin (ILL) in France for simultaneous SAXS/SANS experiments. Compared with an independent experimental approach, the simultaneous SAXS/SANS experimental approach ensures the exact-

ness of the probed samples, especially for time-resolved studies. The SAXS/SANS experimental setup will indispensably permit to instantaneously analyse and understand the complicated correlated nanostructures of two different types of nanoscale components in the same sample volume. For instance, a temporal structural cross-correlation between organic stabilizing agent (cetyltrimethylammonium bromide; CTAB micelles) and gold seeds, which cooperate in the formation of different size/shape of large stabilized gold nanorods during the synthesis process [1] was successfully probed. [1] T. Zech, et.al., Part Part Syst Charact, 39, 2100172, 2022.