

CPP 11: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods

Time: Monday 15:00–16:00

Location: H8

CPP 11.1 Mon 15:00 H8

GISANS sample environment for the investigation of thin polymer films — •TOBIAS WIDMANN¹, LUCAS KREUZER¹, NURI HOHN¹, KUN WANG¹, GAETANO MANGIAPIA², YVONNE HERTLE³, THOMAS HELLEWEG³, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — ²HZG at MLZ, 85748 Garching — ³Bielefeld University, Physical and Biophysical Chemistry, 33615 Bielefeld

The investigation of thin polymer films with neutrons allows a non-destructive probe on their structure and composition. In the framework of the FlexiProb project, which plans an interchangeable sample environment for different neutron experiments at the European spallation source (ESS), we designed a setup for grazing incidence small angle neutron scattering (GISANS). The new sample chamber offers a wide range of adjustable relative humidity with fast switching times. Moreover, a homogeneous heat distribution and reduced condensation of the humid air is realized by a spherical design with fluidic channels inside the chamber walls. A separate gas-mixing and air-flow setup, gives precise control over the air conditions inside the chamber. To demonstrate its options, thin microgel films constituted of thermoresponsive NIPAM with N,N'-methylenebisacrylamide as cross-linkers are placed inside and humidified from 0 to 100 %RH and vice versa. The film response is analyzed with time-of-flight GISANS in order to observe structural changes in the films over the course of the humidification.

CPP 11.2 Mon 15:15 H8

Development of a Sample Environment for in-situ Dynamic Light Scattering in Combination with Small Angle Neutron Scattering for the Investigation of Soft Matter at the European Spallation Source ESS — •ANDREAS SCHMID¹, SEBASTIAN JAKSCH², HENRICH FRIELINGHAUS², TOBIAS SCHRADER², HARALD SCHNEIDER³, and THOMAS HELLEWEG¹ — ¹Physical and Biophysical Chemistry, Bielefeld University, Bielefeld, Germany — ²Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at MLZ, Garching, Germany — ³Scientific Activities Division, FLUCO Platform, European Spallation Source ERIC, Lund, Sweden

The most brilliant and most powerful neutron source in the world, the European Spallation Source ESS, is currently built in Lund. In our project FlexiProb we developed three sample environments for the investigation of soft matter to maximize the potential of the ESS with regard to the very high neutron flux. These are sample environments for small angle neutron scattering (SANS) with in-situ dynamic light scattering (DLS), under grazing incidence (GISANS) and on free-standing liquid films and foams. All sample environments are built on an universal carrier system to ensure a high repeatability and flexibility as well as a minimum switching time between different sample environments. The DLS/SANS module developed in our subproject provides additional control parameters, e.g., the sample stability during the SANS measurements. We developed a special sample holder for about 40 samples which allows the simultaneous measurement of SANS and DLS at two different scattering angles and a precise temperature control.

CPP 11.3 Mon 15:30 H8

Container-free sample environment for neutron scattering — •SEBASTIAN W. KRAUSS¹, RALF SCHWEINS², ANDREAS MAGERL³, and MIRIJAM ZOBEL¹ — ¹University Bayreuth, Bayreuth, Germany — ²Institut Laue Langevin, Grenoble, France — ³Friedrich-Alexander-University Erlangen-Nuremberg, Erlangen, Germany

In-situ small angle X-ray and neutron scattering (SAXS / SANS) provide valuable insights into soft matter systems, such as micelles, biological macromolecules or nanoparticle (NP) formation. For SAXS free-jet setups are established, but the counterpart for SANS was missing, as SANS requires large sample cross sections^[1]. Here, we introduce a novel free-film setup, where the neutrons only penetrate a flowing liquid film optimized to a sample area of 7x10 mm² with a typical film thickness of 0.5 mm as determined from the incoherent scattering of the film. In order to suppress H/D-exchange from the humidity in the air for the operation of the setup with deuterated solvents, we jacketed the setup in a containment filled with Helium. To validate the H/D-ratio over time, three independent methods have been used: IR, gravimetry, incoherent neutron scattering. The main benefit of the free-film is the reduction of the background scattering by 37 % in comparison to measurements in a standard Hellma cell as typically used for SANS. Furthermore, we showcase the setup for the formation of EDTA-capped CdS nanoparticles, in order to investigate the role of the weakly scattering EDTA ligand shell in the nucleation process, having been inaccessible so far.

[1] Lopez, C. G., (2018). J Appl Crystallogr 51, 570-583.

CPP 11.4 Mon 15:45 H8

Gold-labels Enhance Small-angle X-ray Scattering Measurements — •JAN LIPPERT — LMU Munich

SAXS is a powerful tool to probe the structure, interactions and dynamics of biological macromolecules and their complexes in free solution, under virtually arbitrary solution conditions. However, the information content in traditional SAXS measurements is limited, making it impossible to obtain atomic resolution structures from SAXS data alone. To enhance the information content available from standard biological SAXS measurements, we use small (~1.4 nm diameter) gold nanocrystals. The gold nanoparticles can be site-specifically attached to DNA, RNA, and proteins, provide very high scattering contrast in aqueous buffer, and are well suited for ASAXS experiments. We have recently demonstrated two different and complementary schemes to apply gold labels in biological SAXS measurements: As molecular distance rulers in ASAXS measurements [1] and as fiducial markers in standard biological SAXS measurements to provide a sequence-to-low resolutions structure map [2]. Here, I will discuss the possibilities provided by these labelling schemes and given an outlook on how they will be able to provide novel insights into the structure and dynamics of polymers and biological macromolecules in solution. [1] T. Zettl et al., Nano Letters (2016) 16:5353-7. [2] T. Zettl et al., Science Advances (2018) 4:eaar4418.