CPP 2: Focus: Soft Matter and Nanocomposites - New opportunities with advanced neutron sources I

Neutrons are an essential tool in science and research for probing the structure and dynamics of matter from the mesoscale to the nanoscale and from seconds to nanoseconds. To characterize soft matter nanocomposites, nanoparticles and nanomaterials structure and dynamics of such materials can be studied to probe aspects of safety on health and environment of such new materials. Deuterated molecules allow to highlight polymer interactions or interaction of drugs and peptides. Time resolved measurements can follow the self-assembly of colloids to clusters and nano-sized structures or conformational changes in complex biological macromolecules. Neutron scattering methods are versatile to study such aspects in particular with the advent of the new European Spallation Source and future compact accelerator based neutron sources. The supposed focus session will review the possibilities for experiments with neutrons in soft matter and nanocomposites at current and the status of Research and Development on ESS and compact accelerator driven neutron sources. It will discuss the scientific and technical challenges by this new development in neutron access in the German and European scientific landscape. Organized by: Stephan Förster (FZ Jülich), Thomas Gutberlet (FZ Jülich), Peter Müller-Buschbaum (TU München) and Walter Richtering (RWTH Aachen).

Time: Monday 9:30–13:00 Location: ZEU 222

Invited Talk CPP 2.1 Mon 9:30 ZEU 222

The Bright Future for Research with Neutrons in Europe — •Thomas Brückel — Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science, Jülich, Germany

Neutron scattering has proven to be one of the most powerful methods for studying structure and dynamics of condensed matter on atomic lengths and time scales. It is essential to understand processes, phenomena and functionalities in a wide range of materials. In Europe we look forward to the start-up of the most powerful MW spallation neutron source worldwide, the European Spallation Source (ESS). Instruments at ESS will be several orders of magnitude more performant that any existing instruments and will allow entirely new type of experiments. Compact accelerator driven neutron sources (CANS) with high brilliance neutron provision are an attractive option to underpin this future flagship facility. They can provide regional access for science and industry, allow for specialized experiments and provide means for method development and training. The High-Brilliance Neutron Source (HBS) project of the Juelich Centre for Neutron Science (JCNS) will allow construction of a scalable neutron source ranging from a local neutron laboratory to a full-fledged highly competitive user facility with open access and service. A vision for the future use of neutrons in Europe will be presented emphasizing the scientific potential of these novel facilities.

CPP 2.2 Mon 10:00 ZEU 222

Reducing the recording time of neutron spectroscopy measurements to investigate kinetic processes — •Christian Beck[1,2], Marco Grimaldo[1], Felix Roosen-Runge[3], Olga Matsarskaia[1], Frank Schreiber[2], and Tilo Seydel[1] — [1]Institut Laue Langevin, Grenoble, France — [2]University of Tübingen, Germany — [3]Malmö University, Malmö, Sweden

Recent developments at the neutron backscattering spectrometer IN16b (ILL, Grenoble) allow to collect high energy resolution ($\delta E \approx 0.9\mu$eV) measurements at constant non-zero energy transfers, also called fixed window scans (FWS). Full quasi-elastic neutron scattering (QENS) spectra need to be measured for several hours while FWS only need measurement times of several minutes. Different models are established for the analysis of elastic FWS. The approaches for inelastic FWS are limited. The shorter measurement time allows to follow the short-time self-diffusive processes of kinetically changing samples. Here, slowly crystallizing protein solutions were used as a model system. We present different frameworks to analyze these data, extracting generalized mean-squared displacements [1] and global diffusion coefficients and to separate the different hierarchical contributions. The results are compared with analyzed floating average full QENS spectra with a time resolution of 15 min [2]. In addition, time-dependent neutron spin echo measurements, collected on the same systems, offer access to the short-time collective dynamics of the sample. [1] F. Roosen-Runge *et al.*; EPJ Web of Conf. 83, 02015 (2015) [2] C. Beck *et al.*; Cryst. Growth Des.; DOI:10.1021/acs.cgd.9b00858

CPP 2.3 Mon 10:15 ZEU 222

Low Background Instrumentation for Small-Angle Neutron Scattering — •Sebastian Jaksch — Forschungszentrum Jülich GmbH Jülich Centre for Neutron Science, Garching, Germany

Current and future neutron scattering experiments in soft-matter are strongly limited by their signal-to-noise ratio, as this determines the sensitivity for weak scatterers, low contrast conditions as well as spatial resolution at very low Q. Both current and future instruments need to take this into account. Using the example of small-angle neutron scattering (SANS), also under grazing incidence conditions (GISANS), this contribution will give an overview of current developments and challenges in that area. These considerations will be mostly focused on the Small-K Advanced DIffractometer (SKADI)[1] as a future SANS instruments at the ESS, technical considerations on a compact SANS instrument at the High-Brilliance Source[2] as well as measurements at the KWS-1[3] SANS instrument at MLZ, Garching, Germany.

[1]Jaksch, S., Frielinghaus, H., Jestin, J., et al., (2014). Concept for a time-of-flight Small Angle Neutron Scattering instrument at the European Spallation Source. Nucl. Instrum. Methods Phys. Res. A, 762, 22-30.

[2]T. Gutberlet et al., (2019). The Jülich high brilliance neutron source project - Improving access to neutrons. Physica B: Condensed Matter, 570, 345-348.

[3]Feoktystov, A. V., Frielinghaus, H., Jaksch, S. et al. (2015). KWS-1 high-resolution small-angle neutron scattering instrument at JCNS: current state. J. Appl. Crystallogr., 48(1), 61-70.

CPP 2.4 Mon 10:30 ZEU 222

Evanescent wave simulations: challenges and opportunities for the interpretation of grazing incidence scattering experiments — •Tetyana Kyrey[1], Marina Ganeva[1], Judith Witte[2], Regine von Klitzing[3], Stefan Wellert[2], and Olaf Holderer[1] — [1]Forschungszentrum Jülich GmbH, JCNS am MLZ, Germany — [2]TU Berlin, Germany — [3]TU Darmstadt, Germany

Grazing incidence small angle neutron scattering (GISANS) and grazing incidence neutron spin-echo spectrometry (GINSES) are a powerful experimental method for the investigation of the structure and dynamics of adsorbed polymer systems. Neutron scattering provides access to the internal dynamics. Combination of neutron spin-echo spectrometry with grazing incidence geometry opens the possibility to probe dynamics of the polymer system in vicinity to the solid substrate in the time range up to 100 ns. In turn, the usage of the GINSES technique has some peculiarity and, due to the novelty of the method and complexity of the scattering geometry, difficulties in further data analysis appear. In the current work we present how simulations within the Distorted Wave Born Approximation (DWBA) with the BornAgain software can be used for GINSES data treatment and for the preparation to the GINSES experiment. Simultaneously we report on the possible challenges and reefs appearing in choosing the best model and the "wrong" understanding of the roughness parameter. With two showcase examples (a PNIPAM-brush and a PEG-microgel adsorbed on Si-surface), the simulation process as well as the application of the simulations to the GINSES data analysis are presented.

CPP 2.5 Mon 10:45 ZEU 222

ESS Testbeamline V20 - Pilot Experiments for Future Neutron Source — •Oliver Löhmann[1,2], Peter M. Kadletz[2], Regine von Klitzing[1], and Robin Woracek[2] — [1]Technische Universität Darmstadt, Germany — [2]European Spallation Source Lund, Sweden

Neutron scattering studies are important to gain insight into structure and dynamics of soft matter. The European Spallation Source (ESS), the future leading neutron source in Europe located in Lund (Sweden), will provide unprecedented neutron flux and a long pulsed time structure. The technical challenges associated with this together with being a 'green-field-site', triggered the motivation to design and install a dedicated testbeamline (V20) at the Helmholtz-Zentrum Berlin. [1,2]

Between 2015 and 2020, V20 was a dedicated instrument for tests of components and methods, particularly to exploit the unique time structure, and served as an integration platform for ESS technologies. Here, we will present highlights of the work done in the last year including reflectometry and SANS experiments, which are highly important for the soft matter community. Additionally, the data handling and reduction processes will be shown. The investigated concepts and methods will be able to handle both the high flux and variable wavelength resolution.

References:
[1] Woracek et al., Nucl Instrum Meth A, 839 (2016), 102-116
[2] Strobl et al., Nucl Instrum Meth A, 705 (2013), 74-84

CPP 2.6 Mon 11:00 ZEU 222

UppCANs: Bringing neutrons to the users — •Maximilian Wolff — Department for Physics and Astronomy, Uppsala University

Neutrons provide unique and essential tools for research across many disciplines ranging from basic sciences to engineering and studies of heritage artefacts. The present neutron facilities are currently decreasing in number. This overall shortage will not be compensated by ESS offering the best available brilliance but a limited total number of beam days.

Ultra-compact accelerator driven neutron sources (UCANS) can provide small facilities and enable easy accessibility by bringing neutron instruments close to the users. These use modest energy protons (~18 MeV) that impact on a light target. This allows an extremely compact design of the moderators. The small size and optimised source design provide good brilliance at reasonable cost. Dedicated instrumentation can compete in performance with current small to medium size facilities.

I will present a project for UppCANs in Uppsala. When built, this would provide neutrons for 5 to 7 beam ports and offer a broad range of modern capabilities in materials research allowing the community at modest cost to both complete straightforward measurements and prepare to exploit world leading instruments elsewhere.

15 min. break

Invited Talk CPP 2.7 Mon 11:30 ZEU 222

Connecting dynamics and phase behavior of proteins: The neutron perspective — •Frank Schreiber — University of Tuebingen, Germany

We discuss the combination of various neutron scattering techniques to shed light on the dynamics of proteins in aqueous solution. This includes several processes, such as backbone and side-chain fluctuations, interdomain motions, as well as global rotational and translational (i.e. center of mass) diffusion. Since protein dynamics is related to protein function and essential transport processes, a detailed mechanistic understanding and monitoring of protein dynamics in solution is highly desirable. In particular, we connect it to the overall phase behavior in terms of clustering, crowding, crystallization, and phase separation [1], employing a combination of elastic, quasi-elastic, and inelastic scattering [2] as well as complementary techniques. Finally, we comment on future perspectives for experiments at advanced neutron sources. Invaluable contributions by numerous collaborators are gratefully acknowledged.

[1] M. Grimaldo et al., JPCL, 10, 1709 (2019) [2] M. Grimaldo et al., Q. Rev. Biophys., 52, e7, 63 (2019)

CPP 2.8 Mon 12:00 ZEU 222

Protein Denaturing Studied by Neutron Scattering: Static and Dynamic Behaviour — •Olga Matsarskaia[1], Lena Bühl[1,2], Christian Beck[1,2], Felix Roosen-Runge[3], Marco Grimaldo[1], Ralf Schweins[1], Fajun Zhang[2], Tilo Seydel[1], and Frank Schreiber[2] — [1]Institut Laue-Langevin, Grenoble, France — [2]University of Tübingen, Germany — [3]Malmö University, Malmö, Sweden

Studying thermal protein denaturing provides valuable information on structural and dynamic aspects related to protein function. Here, we present a combined study of small-angle and quasielastic neutron scattering (SANS and QENS) to shed light on the denaturing of bovine serum albumin (BSA). To obtain insights into the influence of different parameters on protein denaturing, temperature, crowding and charge screening by NaCl are used as control parameters. SANS allows us to obtain global structural and kinetic information on the systems investigated. In addition, QENS data yield mean-squared displacement (MSD) values [1], describing the diffusive behaviour of BSA throughout denaturing. We observe that, while the pathway towards the denatured state is unchanged in the presence of salt, the dynamics of the denatured state itself changes upon the addition of NaCl. Our results offer a framework for a comprehensive, multi-method characterisation of thermal protein denaturing [2].

[1] Hennig *et al.*, Soft Matter **(8)**, 2012, 1628-1633.
[2] Matsarskaia *et al.*, *in preparation.*

Invited Talk CPP 2.9 Mon 12:15 ZEU 222

Antimicrobial peptides, their mechanisms of action and self-assembly revealed by scattering techniques — Josefine Eilsø Nielsen, Nico König, and •Reidar Lund — Department of Chemistry, University of Oslo, Norway

Antimicrobial peptides are remarkably effective towards a broad spec trum of bacteria and seem to be able to evade much of the resistance mechanisms making their interesting as therapeutics. Their main mode-of action is believed to be through selective interactions with the cytoplasmic membrane, although the microscopic mechanisms is not yet fully understood. Unfortunately, these compounds cannot easily be translated into medical applications due to degradation and hemolysis. However, self-assembly might be a promising strategy to improve the stability. First, we will consider natural antimicrobial peptides and their interactions with model lipid membranes mimicking mammalian and bacterial cells. Using Small-angle X-ray (SAXS) and neutron reflectometry, we extract the location of the peptide and the structure of the lipid bilayer. The lipid dynamics, i.e. flip-flop and molecular exchange, can be deducted using time-resolved SANS . Comparing the structure and the dynamics, we obtain unique microscopic insight into the mode-of-action. In the last part, we present results of a series of de novo designed antimicrobial peptide that assemble into nanosheet-like structures with enhanced in vivo stability. Using results various neutron scattering techniques, we will discuss the 2D/3D assembly, interfacial interactions and dynamic stability of these compounds.

CPP 2.10 Mon 12:45 ZEU 222

Quantifying Nerve fibers in the Brain Section by Small Angle Scattering — •Santanu Maiti[1,2], Henrich Frielinghaus[3], Martin Dulle[1], Markus Axer[2], and Stephan Förster[1] — [1]Jülich Centre of Neutron Science (JCNS-1/ICS-1), Forschungszentrum Jülich GmbH (FZJ), Jülich, Germany — [2]Institute of Neuroscience and Medicine (INM-1), FZJ, Jülich, Germany — [3]Jülich Centre for Neutron Science at MLZ (JCNS-MLZ), FZJ, Garching, Germany

The structure and function of a brain is intricately linked to the structural connectome, i.e. the neurons and their connections [1]. The complete structural map of its nerve fibers and the exact quantification of their constituents is essential to understand the brain function, dys-function and neurodegenerative disease. Here, we map the whole brain section by small angle neutron/x-ray scattering (SANS/SAXS) to investigate the microstructural insights of the neurons [2-4]. We quantify the spatial distribution of the nerve cells and their degree of orientation from the anisotropic scattering signals. We determine also the orientation of myelinated axon and their orientational order over the section from the myelin peak. Finally, we compare them with 3D polarized light imaging (PLI) results to have a complete map of the connectome [5]. In future, the scanning neutron/X-ray imaging can serve as an alternating technique for neuroimaging. [1] C. S. von Bartheld et al, J. Comparative Neurology, 524, 3865 (2016). [2] H. Inouye et al., PLOS One. 9, e100592, (2014). [3] M. Georgiadis et al, NeuroImage, 204, 116214 (2020). [4] S. Foerster et al, Langmuir 31, 11678, (2015). [5] M. Axer et al Front. Neuroinform., 5, 34 (2011).