

canSAS XI workshop

July 8 to 10, 2019 in Freising

Viva Vita

Gartenstrasse 57, 85354 Freising

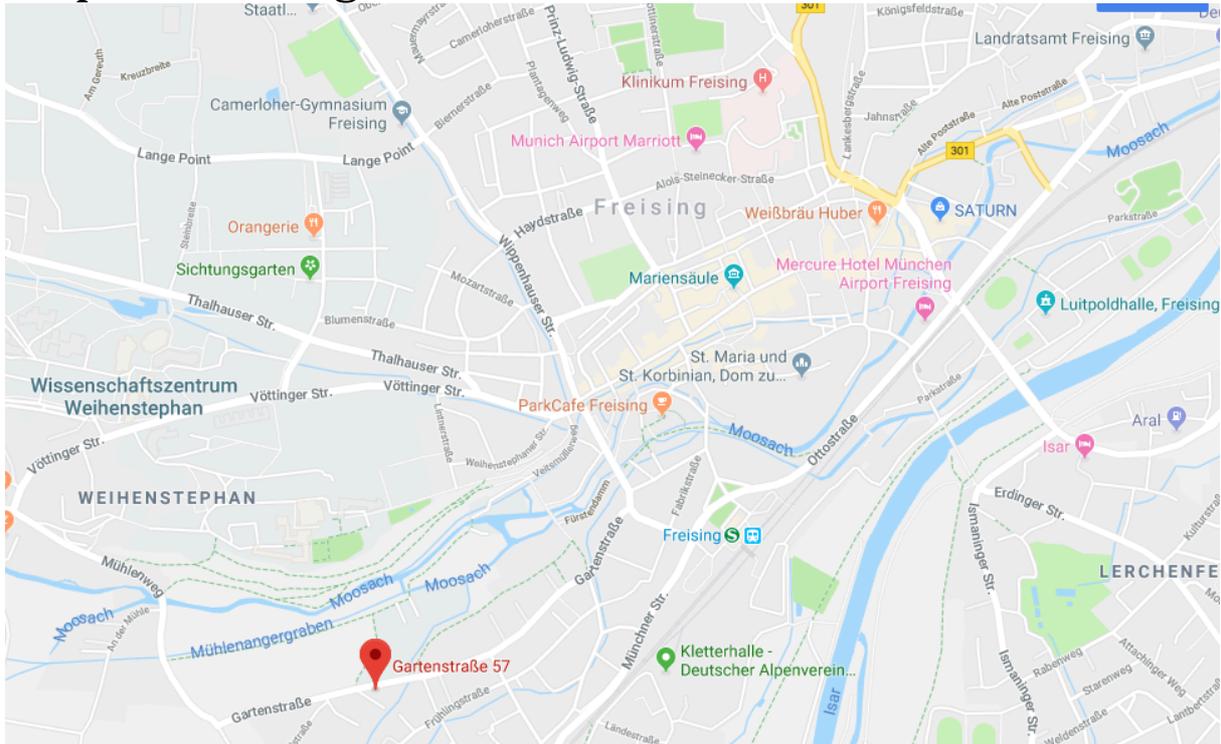


Organizers:

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Map of Freising:



Venue: Viva Vita Freising
Gartenstrasse 57
85354 Freising
Tel.: +49 8161 4830151

Connections from the Airport Munich to Freising

The bus #635 leaving from Terminal 1 (central hall, outside) directly connects to trainstation Freising twice an hour (xx:01 and xx:41). (The terminal 2 stop I never used. The bus leaves there a little earlier.)

The RE train leaving from the airport trainstation directly connects to trainstation Freising 28min past the hour.

Taxis at the airport are not very happy to connect to Freising only (ca. 30€) instead of Munich (ca. 60€). Most friendly taxis are found next to Terminal 1, central hall, opposite to the busstops. Whatever you chose, please sit in the taxi first and give the destination after entering the taxi! Then, the driver is obliged to serve you.

Program of canSAS XI in July 8-11, 2019

Monday, July 8

11:00	REGISTRATION		
12:00	LUNCH		
13:00	PLENARY: WELCOME		
13:10	PLENARY: Short introduction of each participant		
14:30	PLENARY: Lecture on topics of break out session: GISAS		
14:50	PLENARY: Lecture on topics of break out session: Software		
15:10	PLENARY: Lecture on topics of break out session: Reduction / Reconstruction		
15:30	Coffee Break		
16:00	Breakout: GISAS Chair: Eva M. Herzig calibration (Q,I) standardization	Breakout: Software Chair: Paul Butler SASview bio-specific software	Breakout: Reduction/Reconstruction Chair Theyencheri Narayanan Multiple Scatt./Resolution
17:30	PLENARY: Reporting from each group (5min) + discussion		
18:00	PLENARY: Talk by M. Schwartzkopf on "Tackling high data rates in GISAXS: Current status and future challenges"		
18:30	POSTER SESSION on new instrumental developments/ Software/ Sample environment/ etc.		
19:30	DINNER		

Tuesday, July 9

09:00	PLENARY: Lecture on topics of break out session: Sample Environment		
09:20	PLENARY: Lecture on topics of break out session: TOF_SANS		
09:40	PLENARY: Lecture on topics of break out session: Reduction / Reconstruction		
10:00	Breakout: Sample Environment Chair: Katie Weigandt Microfluidics, Rheometers, SEC.....	Breakout: TOF-SANS Chair: A. Sokolova/A. Jackson Data reduction (binning etc.) Detectors	Breakout: extended Q-range Chair: Wim Bouwman SESANS,USANS,VSANS xrays??
10-11h	Coffee will be for own service in parallel to break out sessions		
11:30	PLENARY: Reporting from each group (5min) + discussion		
12:00	LUNCH		
13:00	PLENARY: Lecture on topics of break out session: Dissemination		
13:20	PLENARY: Lecture on topics of break out session: Data Formats		
13:40	PLENARY: Lecture on topics of break out session: Reduction / Reconstruction		
14:00	Breakout: Dissemination Chair: Adrian Rennie Outreach/Collecting Resources for understanding SAS	Breakout: Data formats Chair: Tim Snow (Jemian remote) instrument/samples/... NXcanSAS	Breakout: Reduction/Reconstruction Chair: Sylvain Prévost universality of corrections, bridges between SAXS/SANS, good practice, and techn. dev., uncertainties
15:30	Coffee Break		
16:00	PLENARY: Reporting from each group (5min) + discussion		
16:30	POSTER SESSION on new instrumental developments/ Software/ Sample environment/ etc.		
17:30	TRANSFER / WALK to the Weihenstephan Brewery		
18:15	Brewery tour		
19:00	DINNER		

Wednesday, July 10

09:00	PLENARY: Talk by Roberto Coppola on Steel investigations using SANS	Break out rooms available...
09:30	PLENARY: Talk by Satoshi Koizumi on SANS at the compact neutron source	
10:00	PLENARY: Talk by Yi-Qi Yeh/ U-Ser Jeng on Stoichiometric unfolding of bovine serum albumin	
10:30	Coffee Break	
11:00	PLENARY: General Discussion PLENARY: Wrap up & Actions	
12:00	LUNCH	
13:00	Bus to reactor tour at MLZ	
13:30	Guided reactor tour about FRM-II	
15:30	Bus from MLZ to Airport	

Thursday, July 11

Discussions with Anton Paar on implementing their MCR rheometers to instrument control software

The MLZ tour on Wednesday is meant for everybody. A list on Monday will ask for explicit participation. We leave by bus from Viva Vita. The bus returns to the airport MUC and to Freising city centre.

The Anton Paar tour is for *registered* participants *only*.

On Thursday, July 11, the bus will leave from the train station Freising (S-Bahn station) at 8am. We return to the airport MUC and to Freising city centre.

Abstracts

All abstracts are orderd according to the time within the program. Posters are at the end.

(Eva M. Herzig) Intro Breakout session on GISAS

Grazing incidence scattering

Eva M. HERZIG

Universität Bayreuth, Dynamik und Strukturbildung – Herzig Group, Bayreuth, Germany

Exploiting scattering in a shallow grazing incidence geometry allows to probe a much larger sample volume than for the transmission geometry. Therefore, this technique is particularly suited for extracting length scales within thin films or at interfaces. Since such samples can often be measured as prepared or during preparation and the technique in general does not destroy the samples during measurements, time-resolved measurements are highly attractive. Since synchrotron radiation has gained tremendously in brilliance, these time-resolved measurements can be exploited to study structure formation at interfaces or within thin films. It is therefore possible to track structure formation processes, for example, within printed functional materials [1,2,3].

Apart from calibration issues that should be addressed, we also want to discuss beam damage and how to ensure it is avoided, to obtain reliable time-resolved measurements. We further want to discuss automated and multimodal measurements in combination with grazing incidence scattering (X-rays, neutrons, spectroscopy, etc) and the related software needs.

[1] O. Filonik, E. M. Herzig et al, Energy Technology, 2019, 10.1002/ente.201900343.

[2] S. Pröller, E. M. Herzig et al, Advanced Energy Materials, 2016, 6, 1501580.

[3] S. Pröller, E. M. Herzig et al, Review of Scientific Instruments, 2017, 88, 066101.

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(Paul Butler) Intro Breakout session on Software

Water water everywhere nor any drop to drink

PAUL BUTLER

National Institute of Standards and Technology, Gaithersburg, MD, USA

The rapid advances in sources, instrumentation, and the technique itself promise to revolutionize the output and impact of small angle scattering on materials of ever increasing complexity. In that environment, data analysis tools are currently one of the largest bottlenecks to delivering the potential of these advances, leaving us awash in unanalyzed data. The problem is not that codes don't exist; on the contrary they are legion as evidenced by lists such as can be found on the sas portal (www.smallangles.org//content/Software). Rather, the problem seems to be that the existing tools are limited, not accessible to the regular SAS practitioner, not maintained, much less developed, or only useful for "friends of the author." Further many of these suffer from the "bus syndrome" in that they cease to be even remotely useful once the single author retires or otherwise moves on.

There is a growing recognition that strong computational tools for analysis are on the critical path for delivering science from beamlines and that cybertools in general will be essential to delivering science in the 21st century and beyond (see NSF cyberinfrastructure initiatives, european framework programme support etc). Yet in both cases, progress is limited by the veritable plethora of possibilities and the extremely finite resources. In particular after building new sources and their instrument suites facilities start to struggle with data acquisition, and even more so with reduction, and rarely get far in supporting analysis.

Emerging advanced analysis techniques such as the application of molecular simulations and machine learning to SAS analysis, or "multi-modal" analysis, simultaneously fitting data from a variety of techniques applied to the same sample, hold huge potential for unleashing the promise of the upstream advances. However, these exciting opportunities remain a long way from being generally accessible to the sas practitioner and will require significant and sustained effort and resources. The current heavy interest in these methods is providing a window of opportunity in terms of funding. On the other hand, such a window can also lead to a gold rush mentality with everyone trying to jump into the fray at once posing a real risk that the finite resources will be squandered leading to only marginal advances while starving established packages of the resources to keep them maintained and accessible.

Thus from the point of view of the nomadic sas practitioner, the problem, and also the opportunity, is to maximize the impact of very limited resources compared to the needs/desires and to balance the need for easy to use, robustly supported, maintained and developed packages of standard analysis tools with the need for the development and maturing of new advanced techniques into robust easy to use platforms that are readily accessible to the SAS practitioner. In all cases the tools need to work with reduced SAS data of any origin.

In this brief presentation I will outline some of the issues I have seen and provide some seeds for discussion about possible solutions that can hopefully lead to a productive discussion about the topic such as defining the opportunities, finding new sustainable models for development, and how to capture a maximum share of the limited resources for SAS development and maximize the benefit to the community therefrom.

(Theyencheri Narayanan) Intro Breakout session on Reduction / Reconstruction

Multiple scattering effects at small and ultra small-angle scattering region

Theyencheri Narayanan¹

¹ESRF – The European Synchrotron, Grenoble, 38043 France

This session aims to discuss the different manifestations of multiple scattering by neutrons and X-rays over the small and ultra small-angle range. In particular, subtle multiple scattering effects are difficult to avoid in the ultra small-angle region. We plan to discuss strategies for minimizing multiple scattering and reduce the complication of data analysis. While the static scattering profiles measured by ultra small-angle X-ray scattering show noticeable differences due to multiple scattering, the corresponding dynamics probed by X-ray photon correlation spectroscopy display much less significant deviation [1]. This is similar to observations by light scattering where again the dynamics is less sensitive to multiple scattering.

[1] E.F. Semeraro, J. Moeller and T. Narayanan, *J. Appl. Cryst.*, **51**, 706 (2018).

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(Matthias Schwartzkopf) Evening Talk

Tackling high data rates in GISAXS: Current status and future challenges

Matthias SCHWARTZKOPF¹, Sven-Jannik WÖHNERT¹, André ROTHKIRCH¹, Chenghao LI², Wolfgang WAGERMAIER², Peter FRATZL², Stephan V. ROTH^{1,3}

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In situ and *operando* real-time GISAXS investigation of process kinetics on the nanoscale with high acquisition throughput becoming more and more relevant [1]. The high time resolution in the millisecond regime (e.g. 67 fps) allows for instance the determination of kinetics of initial nucleation and subsequent cluster growth during sputter deposition and enables a precise investigation of gold cluster growth kinetics under conditions advancing towards industrial manufacturing [2]. More than 10,000 GISAXS scattering images respectively several Gbyte raw data per sample is collected during a typical sputter deposition experiment of 150 seconds and can be regard as a kinetic growth movie in reciprocal space. These novel experimental opportunities for tackling scientific questions raise further challenges regarding data analysis of extensive data sets. In this context, a new software package called DPDAK is developed at DESY (Hamburg) in collaboration with MPIKG (Golm), which operates in a user defined plugin framework for specified reduction of huge amount of complex data [3]. The software allows visualizing the evolution of key scattering features in multidimensional data sets [4] in convenient clear presentations as contour plots even in an online-based batch-processing mode. In near future, the rise of even more advanced light sources and much faster detectors with higher pixel density will potentiate the demands on software-based analysis in photon science. In addition, combining the GISAXS setup with complementary methods such as ellipsometry or spectroscopy for determination of structure-properties correlations will further increase the complexity of data analysis [5].

[1] Schwartzkopf, Roth, *Nanomaterials* **6**, 239 (2016).

[2] Schwartzkopf et al., *Nanoscale* **5**, 5053 (2013).

[3] Benecke et al., *J. Appl. Crystallogr.* **47**, 1797 (2014).

[4] Schwartzkopf et al., *ACS Appl. Mater. Interfaces* **9**, 5629 (2017).

[5] Schwartzkopf et al., *ACS Appl. Mater. Interfaces* **7**, 13547 (2015).

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(Kathleen M. Weigandt) Intro Breakout session on Sample Environment

Sample Environment Discussion Primer

Katie Weigandt

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In this talk I will set the stage for discussions regarding sample environment and integration of sample environment with SAS instrumentation. There will be particular emphasis on the development of flow cells and rheoSANS, but general challenges of integrating sample environment with SAS measurements and compatibility of sample environment across facilities will be discussed. What are the major hurdles to developing and sharing sample environment? How do we interact with outside vendors to meet the general community needs? How should facilities balance between sample environment generalization (available at all facilities) vs specialization (experts developing highly specialized sample environments locally)? How can we make it easier for users to use similar sample environments at different facilities? These are just a few of the questions that may be discussed during the sample environment breakout session.

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(Andrew Jackson) Intro Breakout session on TOF-SANS

Approaches to calibration and normalization of complex detector geometries for time-of-flight SANS

Judith HOUSTON¹, Richard HEENAN², Kalliopi KANAKI¹,
Davide RASPINO², **Andrew JACKSON**¹

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²ISIS Neutron and Muon Source, Chilton, UK

In order to make use of the high neutron flux expected at the European Spallation Source, alternatives to ³He based detectors are required. Furthermore, to maximise the benefit of the time-of-flight method, instruments at ESS will make use of a wide angular coverage of detectors. The LoKI SANS instrument is being developed in a collaboration between ESS and STFC and will make use of ¹⁰B based Boron Coated Straws from Proportional Technologies Inc. In order to obtain acceptable efficiencies, these detectors consist of 7 boron coated copper tubes packed within a 1" aluminium tube, with each copper straw wired as a position sensitive detector. On LoKI, these 1" aluminium detector tubes will then be packed into arrays to make detector panels which will be placed in 4-panel banks around the beam at ~1.3 m and ~4 m from the sample, and a single panel bank on a carriage which will move between ~5m and 10 m from the sample.

The arrangement of the detector tubes and straws within each panel, combined with the placement of the detector banks, creates a complex detection geometry that presents challenges for calibration and normalization. To address this we are undertaking a combination of experimental measurements with detector prototypes, and simulations of the detector system using McSTAS and GEANT4.

Here we present our progress towards developing the detector calibration and data processing scheme for LoKI with a view to sharing our experiences with, and benefitting from the knowledge of, the canSAS community. In particular a key topic that that we would like to discuss is standard samples and methods that can be used for Q and intensity calibration of fixed detector panels that sit out of beam.

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(Wim Bouwman) Intro Breakout session on Extended Q-Range / SESANS etc.

Data analysis of SESANS measurements using SasView

Jurrian H. BAKKER, **Wim G. BOUWMAN**

Delft University of Technology, Radiation Science and Technology, Delft, the Netherlands

SESANS measures the SANS of a sample by the Larmor precession of polarized neutrons in magnetic fields with tilted interfaces [1]. This method yields the polarisation which is a Fourier transform of the scattering pattern which is in real space [2]. The early analysis was therefore done by direct calculations of the scattering length density contrast correlation function [3]. This required a lot of calculations to develop and hampered the wider use of the SESANS method.

For SANS a whole zoo of fitting models does exist in software as for example SasView [4] and SasFit [5]. In both programmes a Hankel transform is now included to fit also SESANS measurements. This opens up all the developed SANS models for the SESANS community. In the presentation several examples will be shown of the applications.

[1] M.T. Rekveldt, Nuclear Instruments and Methods in Physics Research Section B, **114**, 366 (1996).

[2] W.G. Bouwman, J. Plomp, V.O. de Haan, W.H. Kraan, A.A. van Well, K. Habicht, T. Keller, M.T. Rekveldt, Nuclear Instruments and Methods in Physics Research A **586** 9 (2008).

[3] R. Andersson, L.F. van Heijkamp, I.M. de Schepper, W.G. Bouwman, J. Appl. Cryst. **41**, 868-885 (2008).

[4] www.sasview.org.

[5] J. Kohlbrecher and A. Studer, J. Appl. Cryst. **50**, 1395 (2017).

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(Adrian Rennie) Intro Breakout session on Dissemination

Information – Overload? Further Needs? Better Provision? For who?

Adrian R. Rennie, Uppsala University, Sweden

It has been recognised for some time that dissemination of information about small-angle scattering is important and a valuable activity for canSAS to help the wider community. The web site at www.smallangle.org is set-up as a portal to provide information that covers news, conferences, facilities, software, as well as links to some teaching material. It is now useful to discuss how this can be updated and improved. There is also a need to identify who can engage in these tasks that are appreciated by many.

There are many ideas for improvements but efforts should reflect needs and consider feasibility. Some questions to be addressed are: how do we help people find material? What new material is needed? How is information best addressed to specific target groups? Can we get wider community involvement? Could instructional videos complement text documents? Would presentations of case studies be helpful?

It will be useful if discussion can lead to a concrete action plan.

(Tim Snow) Intro Breakout session on Data Formats

Data Formats Breakout Session

Chairs: Tim Snow & Pete Jemian

Introductory Talk: Tim Snow

Starting in 1998 the canSAS group coalesced around the idea that a common file format would be advantageous in order to aid the average small angle scattering (SAS) user. After eleven years of debate, work and revision the first version of the canSAS1D XML standard was released in 2009. This marked a significant milestone for the SAS community as, finally, there was a format aside from 3- or 4-column ASCII text that was not only suitable for the storage of SAS data but, crucially, allowed for the inclusion of experimental metadata alongside a reduced I vs. q dataset. Over time, this XML format was extended to provide support for multi-dimensional datasets, detector geometry data, radiation source information, data processing provenance, sample details and other pertinent user contributed details and notes.

Subsequently, following on from the progress made in data storage technologies, it was agreed upon that the next revision of the canSAS standard would embrace the NeXus project platform and, therefore, the HDF5 file format. This led to the formulation and acceptance of the NXcanSAS application definition by the international NeXus committee in 2017. Alongside these activities within the canSAS group, numerous neutron, synchrotron and lab based x-ray sources had also moved to the NeXus standard for the storage of raw data. In a similar vein to the NXcanSAS application definition, the NXsas application definition also facilitates the storage of a multitude of different types of metadata alongside, in this case, raw data. The powerful coupling of a raw and reduced data application definition within the NeXus standard has provided the SAS community a strong base from which to grow.

However, large areas of debate still exist within the scientific community as to why, where and/or how to include information about sample containers, information on sample backgrounds and related datasets from other techniques acquired on the same sample; to name but a few examples. This talk will provide a short overview of what is already in place within the NeXus standard as well as providing some initial thoughts of missing elements from the perspectives of the user, beamline scientist and Machine Learning analyst. Directly following on from this will be an hour long breakout session to discuss topics arising from this presentation as well as any other community thoughts arising on the topic of data formats and storage.

(Sylvain Prevost) Intro Breakout session on Reduction/Reconstruction

Can data reconstruction help obtaining better data from Small Angle Scattering?

Sylvain Prevost

The general process in Small Angle Scattering is stepwise, with data acquisition, data reduction, and possibly data “manipulation”, with the choice of the best background to subtract or the need for merging coefficients between configurations. Afterwards, data analysis is performed with little look backward at the original data and their process; in some fields, programs may even base their analysis on the PDDF obtained via Indirect Fourier Transform of the processed data, disregarding the fit quality of the processed data by splines and ignoring the many mathematical decisions required by IFT.

Meanwhile, facilities are changing their data processing programs (PyFAI for ESRF, Mantid for ILL and many other neutron sources), with no higher ambition than to obtain the same result as pluri-decade old programs (PyFAI increasing the processing speed, while Mantid so far decreases it...).

By experience based on SAXS and SANS, I believe data processing could be significantly improved in particular for “difficult” measurements: high angles, very low angles, very weak signal, very strong scattering probability, very high noise (short acquisitions in series).

The following issues are usually not taken into account: geometrical corrections from the samples and from (thick) containers, geometrical corrections from the detection system, incoherent and coherent scattering probabilities, multiple scattering, effects beyond the first-order Born approximation. In addition, data processing requires at least a dark, a flat field, and proper calibrations (q-range and absolute scale). Error estimates are based purely on Poisson statistics (with difficulties to properly implement dark and flat field uncertainties). Q-resolution is often ignored (always in 2D as far as I know) or approximated (and not evaluated in the same way by different software).

Intuitively, it should be simpler to try and model the simplest 1D curve or 2D pattern that could explain SAS data at all configurations measured, based on an entire dataset (possibly continuously growing and not limited to one beam time) allowing to properly evaluate the flat field (from a good prior knowledge), the mask, the instrumental resolution, and better estimating errors. The “theoretical” data thus obtained can be processed to implement scattering probability (including but not limited to multiple scattering) and geometrical corrections. In addition, noisy 3D datasets (time-series) could also benefit from this “reconstruction”, based on expected smoothness, as is done by IFT. Finally, IFT should be a good starting point to initiate data reconstruction from raw data rather than from processed data.

Of course the reconstructed data should only ever be presented aside the reduced data, and users would still have to make an intelligent evaluation of the goodness of reconstruction.

This scheme would be particularly helpful for a possible multi-beam USANS setup, consisting in spreading on a high-resolution detector a large number of small neutron beams, where cross-talk should be easily added to the reconstruction process.

(Roberto Coppola) Plenary Talk

Reproducibility and Reliability in SANS Measurements of Irradiated Steels for the Future Fusion Reactors

Roberto COPPOLA¹, Artem FEOKTYSTOV², Henrich FRIELINGHAUS², Aurel RADULESCU²

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²FZ-Juelich JCNS at MLZ, Lichtenbergstr. 1, 85747 Garching, Germany

Severe and unprecedented radiation damage effects are expected in structural materials to be utilized in the future fusion reactors: in fact, the exposure to 14 MeV neutron fluxes will produce helium concentrations and damage levels (dpa, displacement per atom) one order of magnitude higher with respect to the fission reactors. SANS provides a powerful experimental tool to investigate such effects, particularly in the ferritic/martensitic steels currently considered as the prime option for the “first-wall” of the future *tokamaks*; furthermore the utilization of polarized beams can provide unique micro-structural information by the nuclear-magnetic interference.

This contribution will discuss recent SANS results, obtained at different neutron sources on the European reference ferritic/martensitic steel Eurofer97/1; the investigated samples had been neutron irradiated at low temperatures, in the dose range 2.5 – 16 dpa, with estimated helium concentrations ranging between 80 and 5600 appm. Reproducibility and reliability issues will be discussed concerning both the comparison of SANS cross-sections obtained for a same sample in different experiments and the metallurgical exploitation of such results by inverse transformation of the SANS data. The comparison with available electron microscopy results will also be discussed.

Recent references:

R. Coppola, M. Klimenkov, A. Möslang, R. Lindau, M. Rieth, M. Valli, *Micro-structural effects of irradiation temperature and helium content in neutron irradiated B-alloyed Eurofer97-1*, Nucl. Mat. En. 17 (2018) 40-47

R. Coppola, M. Klimenkov, *Dose Dependence of Micro-Voids Distributions in Low-Temperature Neutron Irradiated Eurofer97 Steel*, Metals, 2019, 9, 552

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(Satoshi Koizumi) Plenary Talk

Time-of-flight Small-angle Neutron Scattering Using IBARAKI Spectrometer iMATERIA - Ambitious Attempt for Industrial Use -

Koizumi Satoshi

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Based on a powder diffractometer (iMATERIA, BL20) at a pulsed neutron source J-PARC, we newly developed a forward detector to detect small-angle scattering. SANS at the pulse neutron source is characteristics for a time-of-flight (TOF) method, using a wide band of wavelength (λ) from 1 to 10 Å. This wide band of wavelength is combined with different scattering angle (2θ) determined by detector positions, so that a wide q -region (from 0.003 to 40 Å⁻¹) can be immediately covered, where q is a wave number (see definition in Fig.1). We are developing an USANS detector behind the SANS detector, with which we are able to reach to $q < 0.001$ Å⁻¹. Since 2016, we started a user program dedicated especially to industrial use, in order to investigate an industrial product as it exists. Industrial goods are characteristic for a hierarchical structure composed of multi components. In this presentation, we report current activities on iMATERIA. The key words and topics are as follows,

- (1) Hierarchical structure and multi-scale observation from atomic to self-assembled structure length scales, achieved by simultaneous measurement of back scattering and forward small-angle scattering
- (2) Multi component and Contrast variation by dynamic nuclear polarization with 7 tesla super conducting magnet.
- (3) Precise structural analysis on a modelled sample prepared on a flat substrate, by grazing incident scattering reflectivity.

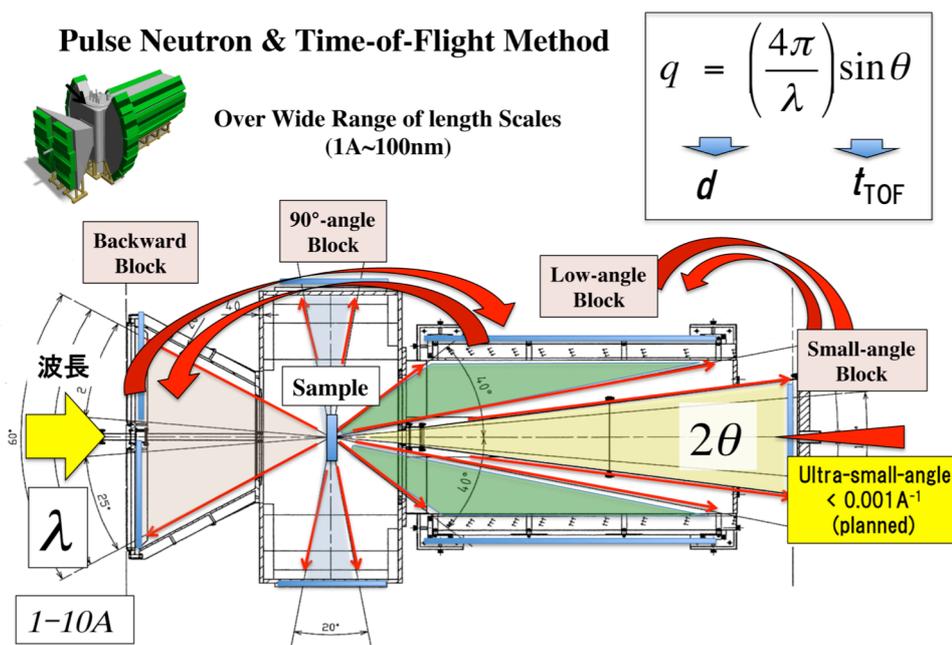


Fig. 1 SANS instrument (iMATERIA, BL20) at a pulsed neutron source J-PARC.

(Yi-Qi Yeh / U-Ser Jeng) Plenary Talk

Stoichiometric unfolding of bovine serum albumin by surfactant, as revealed from HPLC/SAXS with online observation of UV-Vis absorption and refractive index

Yi-Qi. Yeh¹, Kuei-Fen. Liao¹, Orion Shih¹, Wei-Ru Wu¹, Chun-Jen Su¹, U-Ser Jeng^{*1,2}

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Detergents are commonly used to disrupt noncovalent interactions of proteins, leading to detergent-protein complex or stabilized recombinant proteins. In past, many methods have been used to investigate conformational changes of proteins and protein-detergent complexes to understand their interactions, polarity and stability in varied detergent concentrations. The local structure of such protein/detergent complex could be resolved by spectroscopies; however, resolving the corresponding stoichiometric protein unfolding conformation requires separating the effects contributed by the coexisted protein/detergent complex and SDS micelles in the solution.

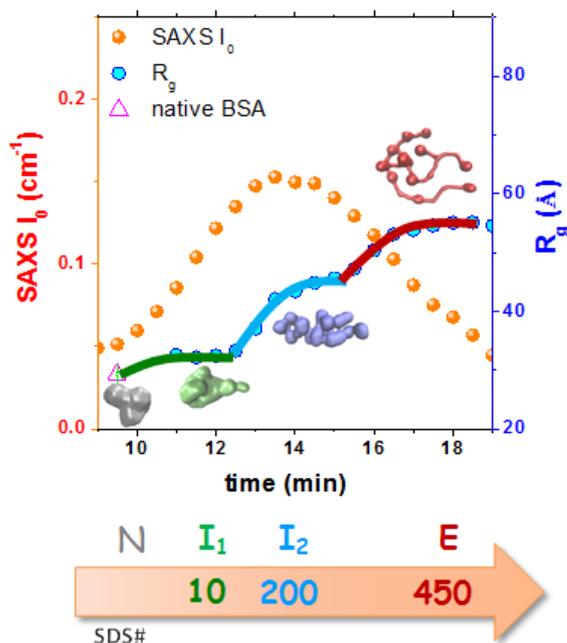


Figure 1. R_g and I_0 profiles extracted from the SAXS data measured along the chromatogram $I_{UV\ 280nm}$ of the BSA/SDS solution in SDS buffer.

In this work, we show that sodium dodecyl sulfate (SDS), a frequently used surfactant in purification of membrane proteins, can bind to bovine serum albumin (BSA) for multistage unfolding. The on-line protein purification system of high performance liquid chromatography (SEC-HPLC) incorporated to the beamline 23A synchrotron small-angle X-ray scattering (SAXS) instrument of the Taiwan Light Source at NSRRC, allows separating the scattering contributions from the BSA/SDS complexes and SDS micelles. Together with integrated observations of UV-vis absorption and refractive index (RI), we have resolved the stoichiometric unfolding conformations of BSA by SDS monomers to micelles. In Figure 1, the corresponding protein-SDS association numbers along the unfolding process are determined uniquely from a combined analysis of UV-Vis absorption, refractive index, and zero-angle SAXS intensity measured in one sample elution.

[1] Yeh, Y.Q. et al., J. Phys. Chem. Lett. **8**, 470–477 (2017).

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(Peter Boesecke) Poster Session, Poster #1

Data treatment and data storage at the TRUSAXS beamline ID02 in 2020 after the EBS upgrade of the ESRF storage ring.

Peter BOESECKE

European Synchrotron Radiation Facility, Grenoble, France

During 2019 the storage ring of the ESRF is physically replaced with a new structure called EBS, extremely brilliant source. It will provide a synchrotron beam with a 40-times higher spectral brilliance than before (<https://ebs.esrf.fr/news/>). The down time at the beamlines is used for replacing existing control and acquisition tools and taking action for implementing the ESRF data policy which has the objective of regulating the ownership of experimental data, e.g. for making it available to the public after an embargo period.

The new control system, BLISS, an ESRF inhouse development, is based on the popular programming language Python. Together with existing Python tools provided by the ESRF data analysis unit (silx, pyFAI, FabIO, see <https://www.silx.org/>) we are planning at ID02 [1] a modern, user-friendly beamline environment for storing experiment data in HDF5-NEXUS files and employing local metadata catalogues (ICAT) for documentation and data mining.

The upgrade is a major challenge and the consequences will impact all researchers at ID02.

For facilitating the integration into the new Python environment we are currently upgrading our inhouse software tools, e.g. saxsutilities (<https://www.saxsutilities.eu/>). The existing small-angle scattering data of ID02, which are mainly saved as ESRF data format (EDF) files, will remain directly readable via the FabIO Python interface. Programs that are currently used in our data processing pipelines will be kept operational in the future, at least for data-files written at ID02.

We will continue of saving descriptive metadata together with scattering data in a single data file (see CANSAS I, 1998). This method allows analyzing 2D scattering data step by step because the metadata values in the output files are consistently updated. Such files can be reused as input for further calculations. Descriptive metadata must not be confused with beamline metadata, e.g. motor positions or the storage ring status: these metadata describe the state at the time of acquisition and must therefore not be changed. Descriptive metadata are typically initialized with beamline metadata, e.g. wavelength, but they can be refined during data reduction.

The problems and challenges of migrating to the new control system and data format will be presented. It seems today unrealistic that the new control software (BLISS) will be already fully available at the restart of ID02 in spring 2020. However, using ICAT and writing raw data as HDF5/NEXUS files should be a realistic vision.

[1] Narayanan, et al., Journal of Applied Crystallography, **51**, 1511 (2018)
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(Sebastian Jaksch) Poster Session, Poster #2

SANS calibration, data reduction and reconstruction

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It is indispensable to achieve excellent calibration for the scattering angles and the recorded intensities in order to achieve data that can both be treated reliably as well as be compared when measuring at several different instruments. Only having data available that is reliable in that way allows a reasonable reconstruction of the sample structure.

In this contribution we are going to discuss several factors that impact this calibration and the subsequent data reduction from a technical standpoint. This includes, but is not limited to the achievable limits for calibration and the incurred errors during the calibration as well as the impact of instrumental features on the calibration.

Since most neutron scattering instruments are scattered far and wide across the world with no direct physical connection apart from the scientists travelling between them also the question of reliable and reproducible standards is important in this consideration. Several standards, some of them secondary round-robin standards have already been established, but often are only either exchanged between a few institutes and/or are hard to reproduce in another place, when the round robin is unavailable or even destroyed over time.

Taking all these features together we are going to discuss the practical implications based on a well-established instrument, the KWS1 [1] at the MLZ in Garching, Germany, where even the comparison of two different detector systems is available and a future TOF instrument, SKADI [2] at the ESS, Lund, Sweden. Based on those two use-cases the advantages and issues of several calibration, reduction and secondary standard systems can be examined in detail.

[1] Artem V Feoktystov, Henrich Frielinghaus, Sebastian Jaksch et al., *Journal of Applied Crystallography*, **48**, 61, 2015.

[2] Sebastian Jaksch, Henrich Frielinghaus et al., *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, **762**, 22, 2014.

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(Adam Washington) Poster Session, Poster #3

SES: A file format for Spin-Echo Small Angle Neutron Scattering

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Spin-Echo Small Angle Neutron Scattering (SESANS) is a recent neutron scattering technique for probing materials. By encoding the neutron's trajectory into its polarization via Larmor precession, the technique is capable of probing length scales on the order tens of microns. Additionally, the technique directly provides real-space correlations, as opposed to the reciprocal space correlations of most scattering techniques, providing complementary information that can elucidate features that can be hidden in the transformed state (e.g. structure factors). The unique properties of SESANS were not well suited by existing file formats. Furthermore, as more SESANS instrument came online and a growing community of users needed to process their data, an interchange format became necessary.

The SES file format is an extensible file format for the storage and exchange of SESANS data. It defines a minimal viable data set in order for the measurement to be processed, but also allows for additional data and metadata to be added on a per-instrument or per-measurement basis. A formal grammar specification has been written for the file format both to allow implementers to verify the validity of their work as well enabling the use of common parser generators to automate implementations.

A small suite of tools has also been developed for processing the file format. This utility, called sestool, allows for data files to be combined, filtered, rescale, or converted. The code is openly available under a BSD license and can run on all major desktop platforms. The development of the tool, written in the pure functional language Haskell, also provided guidance and feedback toward the structure of the formal grammar, ensuring that edge cases in the development of the grammar were properly handled.

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(Chun-Jen Su) Poster Session, Poster #4

Developing Simultaneous Grazing-Incidence Small- and Wide-Angle X-ray Scattering with UV-vis Reflectance Detecting for Thin Film Formation Kinetics during Spin-Coating

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At the 23A beamline of the Taiwan Light Source at the National Synchrotron Radiation Research Center, an on-line spin-coating system is integrated to time-resolved grazing incidence small- and wide-angle X-ray scattering (GISAXS/GIWAXS) together with UV-Vis reflectance detection, for monitoring thin film structural development during spin-coating. With the integrated instrument covering from atomic, to nanometer, and to micrometer length scale, we have observed correlated developments in crystallization, nanodomain formation, and film thinning, of a polymer/fullerene mixture during spin-coating. Our results unveil a vertical liquid-liquid phase separation over the transition from the solution flow-off to evaporation-dominance, leading to a surface layering structure in the early stage of the spin-coating. Based on the structural kinetics deduced, we suggest that shear-enhanced solvent evaporation can supersaturate the surface layer and drive the trapped and molecularly dispersed polymer and fullerenes to demix locally; this leads to comparable crystallization and diffusion kinetics for mutually confined and intercalated nanodomains of surface-oriented polymer crystallites and fullerene aggregates. Integration and calibration of the measurements will be elaborated in the presentation.

[1] W.-R. Wu, C.-J. Su,^{*} W.-T. Chuang, Y.-C. Huang, P.-W. Yang, P.-C. Lin, C.-Y. Chen, T.-Y. Yang, A.-C. Su, K.-H. Wei, C.-M. Liu, and U. Jeng^{*}, *Adv. Energy Mater.* 7 (2017) 1601842(11).

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(Andreas Ulbricht) Poster Session, Poster #6

Characterization of irradiation-induced microstructure in reactor pressure vessel steels

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SANS contributed significantly to the understanding of the behaviour of reactor pressure vessel (RPV) steels exposed to irradiation with fast neutrons. It allows macroscopically representative, statistically reliable and robust measures of size, volume fraction and number density of nm-sized solute clusters to be obtained. In particular, the use of the ferromagnetic properties of the matrix allows, under certain assumptions, the exact determination of the scattering contrast and thus the absolute volume fraction. The lower detection limit in terms of volume fraction is typically about 0.005%. The A-ratio, that is the total-to-nuclear scattering ratio, can be used as one-parameter signature of the mean composition of irradiation-induced clusters. Major limitations of SANS are related to the uncertainty of the scattering contrast (cluster composition, magnetism) and to the lower detection limit. Especially because of the incoherent scattering contribution of different iron isotopes, the lower detection limit is approximately 0.5 nm in terms of radius. The unirradiated reference condition of a RPV steel exhibits a high scattering background essentially caused by different sizes of carbides and should be carefully subtracted from the investigated neutron-damaged condition.

In the present work we give an overview about major influence factors on irradiation-induced microstructural changes. Increase of neutron exposure gives rise to an increase of the volume fraction of solute clusters. This susceptibility is essentially determined by the existing alloying elements and impurities. Cu-rich precipitates are the dominant type of nanofeatures in Cu-bearing steels (Cu > 0.1wt%) and Mn-Ni-(Si) precipitates or their nonequilibrium precursors are the dominant type of nanofeatures in low-Cu, Mn-Ni-alloyed ferritic materials. The size of clusters remains small and does not exceed a radius of 4 nm. In recent years, research was focussed on the transferability from accelerated irradiations to real operation conditions of materials in a power reactor, for instance the effect of neutron flux on irradiation-induced damage. Here, SANS results show a clear trend. The size distribution of low flux condition is shifted towards larger radii. The effect of neutron flux on the volume fraction of irradiation-induced clusters is not so obvious. There seems to be a trend that the cluster volume fraction decreases at increasing flux. Here, the detection limits of SANS (very small clusters and/or reduced scattering contrast) and the uncertainties of the irradiation conditions possibly hide an explicit flux dependence. Differences in the A-ratio were not observed for flux pairs of one and the same material. Thus, no significant changes of cluster composition appear at different fluxes.

Strong and robust correlations between SANS-based characteristics of irradiation-induced clusters, such as (the square-root of) volume fraction and irradiation-induced changes of mechanical properties, such as Vickers hardness, yield stress or brittle/ductile transition temperature are confirmed.

(Wei-Tsung Chuang) Poster Session, Poster #7

Probing the Structural Evolution of Self-assembly Dendron-Jacketed Block Copolymers Using in-situ SAXS

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Hierarchical self-assembled structures and their structural evolution of a series of dendron-jacketed block copolymers (DJBCPs) have been symmetrically investigated by small- and wide-angle X-ray scattering (SWAXS) and transmission electron microscopic (TEM) images. The DJBCP is composed of amphiphilic dendrons, selectively incorporated into the P4VP block of poly(styrene)-*block*-poly(4-vinylpyridine) (PS-*b*-P4VP) *via* hydrogen bonds. Helical-*within*-helical superstructures have been discovered for the first time in an achiral DJBCP system. Evidenced by in-situ SAXS, stretching followed by thermal annealing enables the dendron-jacketed blocks to exhibit several liquid crystal phases with increasingly better packing strength, from smectic to a hexagonally-packed columnar phase; thereby, the global structure of the supramolecular DJBCP complex evolves from body-centered-cubic (BCC), to face-centered-cubic (FCC), then highly oriented tetragonally perforated layer (TPL) structure. Furthermore, we also demonstrated that the formation of perpendicular cylinders on substrates, which resulted from the epitaxial growth from $Im\bar{3}m$ to $P6mm$ *via* $R\bar{3}m$ during the thermal annealing of DJBCP films evidenced by GISAXS. Realizing the structural characteristics of DJBCP self-assembly allow us to control the orientation of cylinders (perpendicular or parallel), and film thickness (from few decade nanometer to few micrometer).

[1] W. T. Chuang *et al*, *ACS Appl. Mater. Interfaces*, 8, 33221 (2016).

[2] W. T. Chuang *et al*, *Macromolecules*, 47, 6047 (2014).

[3] W. T. Chuang *et al*, *Soft Matter*, 2012, 8, 11163 (2012).

[4] W. T. Chuang *et al*, *Chem. Mater.*, 21, 975 (2009).

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(Anna Sokolova) Poster Session, Poster #8

Reactor-based time-of-flight SANS instrument BILBY: accumulated experience in collecting scattering from samples of various nature, dealing with incoherent backgrounds and complex transmissions along with solving issues in non-trivial data reduction

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Australian Nuclear Science and Technology Organization (ANSTO) for more than ten years successfully operates first Small Angle Neutron Scattering instrument QUOKKA [1] and in January of year 2016 commenced user operation of the second SANS instrument, BILBY [2]. The inspiration for BILBY is the D33 machine located at the Institut Laue-Langevin [3]. Similar to D33, BILBY exploits neutron time-of-flight to extend the measurable Q-range, above what is possible on a conventional reactor-based monochromatic SANS instrument.

BILBY has been designed to operate in two different modes: monochromatic mode, where a neutron velocity selector (NVS) filters neutrons of a defined wavelength (from 4.5-30Å) and resolution ($\Delta\lambda/\lambda \sim 10\%$); and in time-of-flight (ToF) mode, where four choppers are used to create neutron pulses at tunable resolution in the range between 3% and 30%. Two arrays of position sensitive tube detectors in combination with available wavelengths from $\sim 2\text{\AA}$ to $\sim 18\text{\AA}$ provide capability to collect scattering data on the wide angular range without changing the experimental set-up.

Taking into account the main focus of the CanSAS meetings, main attention of my presentation will be given to a complexity of ToF mode as such, especially of the ToF data reduction. We have collected an extensive set of scattering data from samples with high content of hydrogen. We will share our ways of dealing with issues caused by inelastic and elastic incoherent background. As one knows, this is the hot topic and one of the major well-knowns problem appearing in data reduction collected on ToF SANS machines. Also we will touch on the subject of the data reduction also giving attention to study samples with complex transmission vs wavelength dependence and to those prone to generating multiple scattering.

[1] K.Wood et al, J. Appl. Crystallogr. **51**, 294-341 (2018).

[2] A. Sokolova et al, J. Appl. Crystallogr. **52**, 1-12 (2019).

[3] C.D. Dewhurst et al, J. Appl. Crystallogr. **49**, 1-14 (2016).

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(Sven-Jannik Wöhnert) Poster Session, Poster #9

dpdak - x-ray analysis software: release 1.4 and current development

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X-ray scattering experiments at modern synchrotron beamlines use high frame rates and yield an increasing amount of data using multiple two-dimensional detectors. DPDAK (directly programmable data analysis kit) offers a way to reduce, process, and analyze such multidimensional datasets [1]. Experiments using combined SAXS and WAXS geometries, as well as with grazing incidence are processed with a tailored plugin-base work tree [2]. This allows the user easily to adapt DPDAK for individual data processing.

Furthermore, DPDAK involves calibration and correction of raw data, integration and extraction of data, creation of mask files, conversion of the data to graphics for publications and many more features. These functionalities can be realized ex-situ after measurements as well as in-situ parallel to the experiment for instant evaluation of data. Five years after the first release the collaboration between the groups from Hamburg and Golm is happy to announce the new version of DPDAK [3]. Basic plugins were revised and new functionalities were introduced. Also new packages specialized on the requirements of specific beamlines (e.g. P03 [4]) were created. We will present the changes and new possibilities of DPDAK 1.4.

References

[1] G. Benecke et al., J. Appl. Cryst. 47 1797. (2014)

[2] Schwartzkopf, Roth, Nanomaterials **6**, 239 (2016).

[3] dpdak.desy.de

[4] https://stash.desy.de/projects/DPDAK/repos/user_minaxs/

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(Adam Engberg) Poster Session, Poster #10

NURF - optimisation of multiple in situ simultaneous, autonomous characterisation techniques with small-angle neutron scattering

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To increase the utility of SANS data, complementary information from other characterization techniques can give a more complete picture of the different aspects of the systems being studied. There is also a growing need for high throughput capability to utilize the high flux neutron sources being built, e.g. at ESS. Therefore, we are developing a platform that enables additional measurements to be performed in situ, as well as automated mixing and filling of a flow-through cell.

The current system allows for UV/vis and fluorescent spectroscopic methods to be applied, as well as temperature control and data logging. This is achieved with a combined flow cell holder and fibreoptic manifold produced by additive manufacturing and incorporates 6 additional probe ports that could be utilized for Raman spectroscopy, camera inspection or other ancillary equipment. A density meter can be connected in-line to provide further additional information. Sample delivery equipment such as HPLC-pumps, coupled to multiple valves makes it possible to achieve automatic cleaning of the flow cell and sample loading, increasing the throughput and utilizing beamtime more efficiently.

These developments open the possibility for broader and more efficient data collection which could be applicable to a range of systems normally studied by SANS.

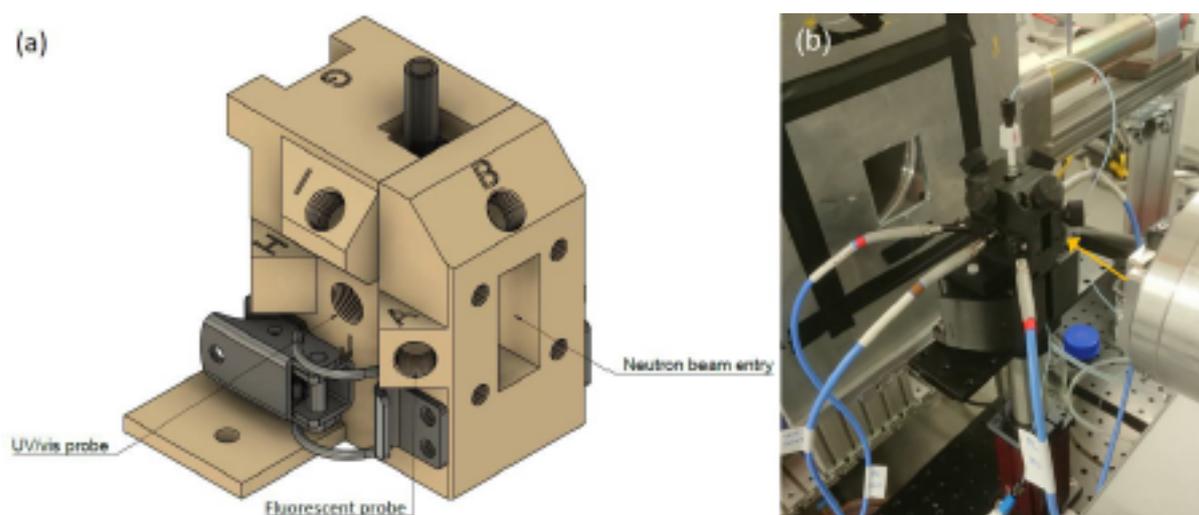


Figure 1. (a) Computer aided design (CAD) drawing of combined flow cell mount and fibreoptic manifold. (b) Setup installed at Larmor, ISIS, with UV/vis and fluorescence measurement equipment installed.

(Yen-Chih Huang) Poster Session, Poster #11

Estimation of fiber theoretical modulus using S/WAXS with *in-situ* uniaxial tensile examination

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Fiber theoretical modulus, which is the elastic modulus of crystal region in a fiber, is the highest modulus of a fiber could possess theoretically. [1-3] Beyond being a modulus ceiling that a fiber could achieve during the manufacturing process, the crystal moduli along the different directions of fiber also provide structural information inside the fiber. The crystal moduli parallel (E_c) and perpendicular (E_t) to the chain axis are correlated to the skeletal conformation, deformation mechanism and the intermolecular interactions as well as the anisotropies respectively. In this study, the theoretical modulus of Kevlar-related fibers were estimated through synchrotron S/WAXS with *in-situ* uniaxial tensile examination. The crystalline and amorphous region in the fiber were assumed to have the arrangement as a series model in which the tensile stress apply homogeneously on the fiber. As the result, the deformation of crystalline region in the fiber could be deduced from the S/WAXS profiles and then the elastic modulus of crystal region can be estimated. [4] The estimated theoretical moduli of Kevlar fibers as reference were quite similar to the reported values, and the experiment results implied that there might be a certain distribution of inter-molecular interaction according to the modulus perpendicular to chain axis (E_t).

[1] S. Lee *et al.*, Polymer, **138**, 124-131 (2018).

[2] K. Nakamae *et al.*, Polymer, **19**, 451-459 (1987).

[3] K. Tashiro *et al.*, Polymer, **29**, 1768-1778 (1987).

[4] W. J. Dulmage *et al.*, Journal of Polymer Science, **28**, 275-284 (1958).

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(L.C. Chiang) Poster Session, Poster #12

The Equipment Control System of the Biological Small-Angle X-ray Scattering Beamline at Taiwan Photon Source

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One of the beamlines at Taiwan Photon Source (TPS), numbered as TPS 13A, is for Biological Small-Angle X-ray Scattering experiments. The main optical components include a double crystal/double multilayer monochromator, a Kirkpatrick-Baez mirror, a vertical deflection mirror, and a four bounce crystal collimator. Various diagnosis equipment are included to help monitoring the status of synchrotron radiation. Four-blade slits constrain the beam size and block unwanted noise. Current amplifiers attached to the slits are used as beam position monitors. At critical locations, there are special beam position monitors designed to be precise in the range of sub-micron to nanometer, which can be used to do continuous monitoring and auto-correction. In front or at rear of some optical components which can change the direction of the x-ray beam, there are fluorescent screens and cameras to observe positions and strength of the beam. Most equipment need electronic motors or high-pressure air to be movable and controllable from a remote control system. With one central integrated control system for all equipment, it will be easier for the scientists to operate the beamline, adjust the conditions of various parameters, do the commissioning, and concentrate on the experiments at hand.

[1] N. R. Hajizadeh, D. Franke* and D. I. Svergun*, J. Synchrotron Rad. **25**, 906–914 (2018).

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(Grethe Jensen) Poster Session, Poster #13

Intermediary companies for industrial neutron and synchrotron measurements

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The huge public investments into large-scale research infrastructures have created a political demand for improved industrial access to measurements at synchrotron and neutron facilities. Especially so in Denmark where 3 billion DKK is being invested in the establishment of the European Spallation Source in Lund, Sweden. It remains an open question how to setup the optimal industrial user structures that will make neutrons and synchrotron investigations more accessible for industry.

So-called commercial intermediary companies present a very overlooked access mode for industry. The access has been identified in recent ESRFI reports [European Strategy Forum on Research Infrastructures Scripta Volume 2: "Long-Term Sustainability of Research Infrastructures", 2017]. These companies specialise in providing commercial services based on measurements at, mainly, synchrotron facilities. So far, little analytical work has been made on understanding and mapping out these companies and their interactions with the facilities and universities.

Ca. 8-10 such entities exist around Europa, and two of them, CR Competence and Saromics, are located in Lund with a close relation to the MAXLAB synchrotron. Similar companies are located at some (but not all) of the synchrotrons around Europe. In the context of the European project "CAROTS", DTI is setting up a network of intermediary companies and will investigate the optimal operational structures and synergetic areas of coordination and collaboration. Many larger companies prefer to use intermediary companies simply due to contractual challenges when dealing with public bodies such as facilities and universities. Also, the intermediary structure resembles the normal business-to-business interaction seen in other more matured service areas.

Initial interviews with the intermediaries point towards potential areas of collaborations being:

- booking of joint beamtimes,
- helping facilities develop a platform to meet and service intermediaries,
- create joint marketing platform,
- technical training workshops for intermediaries,
- definition of common standards for measurement and data protocols.

The network of intermediaries will be setup during autumn 2019 and matured in a series of events in 2020. At the DANSCATT meeting, DTI will present the initial results and the timeline and engage other stakeholders in discussions and potential future collaborations.

(U-Ser Jeng) Poster Session, Poster #14

A Frontier **B**iological **S**mall- and **W**ide-**A**ngle X-ray Scatteri**N**g Beamline for Biological Structures and Biomedical Applications

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During the past ten years, biological small-angle X-ray scattering beamlines were built in nearly all advanced synchrotron facilities worldwide. The consequent impact on the research of structural biology has been well demonstrated with the fruitful results published in high-impact journals. Following this trend, a dedicated, state-of-the-art **B**iological **S**mall- and **W**ide-**A**ngle scatteri**N**g (BioSWAN) beamline at the Taiwan Photon Source (TPS) of National Synchrotron Radiation Research Center (NSRRC) was proposed by Professors. Meng-Chiao Joseph Ho and Ming-Daw Tsai in 2014, which develops into a joint project between the NSRRC and Academia Sinica. With high flux of 5×10^{14} photon/s, versatile optics design, rich environmental controls and in situ complementary detecting, this dedicated TPS BioSWAN beamline aims for advanced biostructural researches and biomedical industrial applications using the following operation modes:

- (1) High flux mode for integrated measurements of SAXS/WAXS/UV-Vis-absorption/Refractive-index(RI)/Multi-angle-light-scattering (MALLS) with online high-performance liquid chromatography (HPLC), suitable for exploring biomacromolecular solution structures of a wide length scale (from Å to μm) and structural kinetics down to microsecond time scale.
- (2) Ultra SAXS (USAXS) mode for resolving hierarchical structures of biomachinery assembly up to 1-μm length scale.
- (3) Anomalous SAXS (ASAXS) mode for metal or mineral distributions (including calcium) in bio organelle or drug carriers.
- (4) Microbeam SAXS/WAXS (μSAXS) mode for structural mapping of the textures or specific infected cells, natural/synthetic bio-tissues, organelles, fibrils, membranes, or biomaterials.

The frontier TPS 13A BioSAXS beamline, expected to be operational in the Spring of 2020, would cover both the needs of academic research and biomedical industrial applications.

PS: The beamline progress is constantly updated in the Facebook BIOSWAN
<https://www.facebook.com/groups/235104753597992/?ref=ts&fref=ts>.

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