

ESS Science Symposium: "Surface and Interface Reconstruction: A Challenge for Neutron Reflectometry"

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Organizers: W. Kreuzpaintner, Th. Gutberlet, H. Wacklin, P. Böni

Surfaces and interfaces are some of the most important topics in contemporary condensed matter research, chemistry, materials research and life sciences. The requirements for research in this field with focus on the availability of more intense neutron beams at new spallation neutron sources (SNS, J-PARC, ESS) and the development of novel concepts for neutron reflectometers were the topic of the workshop.

Wed. 24 Sept. 2014:

Scientifically, the workshop started with a session on structures, structured surfaces and surface reconstruction. Talks were given by Tilo Baumbach, (KIT), Julian Stangl (JKU Linz), Martin Kreuzer (ICN2), Mary Wood and Kathryn Browning (both Cambridge University), presenting current research in the fields of nanostructured surfaces and copolymer templates which all apply grazing incidence and co-planar off-specular scattering techniques. Although the use of synchrotron radiation was emphasized in these talks, they clearly outlined the challenges for the application of future neutron scattering and synchrotron radiation techniques and their complementary use in investigating (magnetic) nano- and complex soft matter structures.

These challenges for off-specular neutron scattering as complementary techniques for synchrotron radiation were discussed in the following discussion session "The role of neutrons and X-rays -- where are the biggest advantages to be gained for each?", chaired by Prof. H. Zabel. In a vivid discussion, the advantages of (co-planar off-specular) polarized neutron reflectivity and GISANS over the corresponding x-ray techniques (XRR, GISAXS), which consist in H-D contrast and other isotopic contrasts as well as larger penetration depth, oxygen sensitivity, the transmission of a neutron beam through a water bath (for investigations of interfaces with water) or the transmission through a thick Si block etc., was spelled out and emphasized. It was also stated that in the future, more and more nanostructured and increasingly smaller samples will be investigated, which, however, currently has the momentum with synchrotron techniques and is a great challenge for neutron scattering. In this discussion, the wish for a user friendly software for (off-)specular data evaluation was also strongly addressed. This wish/requirement was repeatedly mentioned and emphasized within every discussion session of the workshop. The discussion, however, also drifted from the original topic of complementarities of both techniques towards the requirements and wishes for neutron reflectometers at ESS, for which the common knowledge base was not yet presented. It was, hence, agreed upon that Hanna Wacklin will briefly introduce the concept of ESS reflectometers for liquids and solid systems on the following day before the start of the originally scheduled program, such that these aspects could be discussed in more detail in the discussion sessions. It is to note that general discussions in smaller self-organized groups were quite vividly continued between the workshop participants during and after dinner until approximately midnight.

Thu. 25 Sept. 2014:

Thursday's morning session started with a brief introduction on the concepts of the ESS reflectometers FREIA (horizontal, soft matter, life sciences) and ESTIA (vertical, solid matter, magnetism), given by Hanna Wacklin, who updated the audience to a common knowledge base for further discussions. Also SANS setups like LOKI and SKADI were briefly addressed as well as further concepts like spin-echo labelling or the reflectometer design of VERITAS. This was then followed by talks in the field of solid-liquid interfaces and porous interfaces, presented by Stuart Clarke (Cambridge University), Max Wolff (University Uppsala), Peter Müller-Buschbaum (TUM) and Oliver Seeck (DESY), which mainly addressed the investigation of adsorption processes using different scattering geometries, (time resolved) GISANS and general scattering from soft matter interfaces.

After lunch Björgvin Hjörvarsson opened the afternoon session on magnetic structures and interfaces by pointing out the different length scales addressed by scattering techniques. He emphasized the importance of investigating nanostructured surfaces in the future. This was followed by a talk by Brian Maranville, who presented research on Skyrmion lattices -- a new state of magnetic matter that was first unraveled by neutron scattering ahead of other analytical techniques.

The talks were then followed by a discussion session on the topic "Scientific challenges -- what do we want to do in 10 years from now in surface scattering?", which was chaired by Peter Müller-Buschbaum (TUM). The participants quickly agreed that foreseeing the future by 10 years would be a difficult task, but instead a discussion evolved around the question what "could" possibly be the center of interest in the future. By extrapolating the evolution since the 1970's, when the preparation of well defined thin films was still a challenge, through the 1980-1990's, when multilayer/superlattices were a hot topic, through the 2000's (lateral structures) and 2010's (coupled systems, dynamics, magnetism & biology), it was agreed that by the 2020's mainly heterostructures or 2 and 3 dimensionally patterned systems will be investigated in both soft- and condensed matter research, especially also with a view on how structures and functions are linked and how surface dynamical properties can be analyzed. Again, the fact that no standard analysis software is available was mentioned and the requirement for using ESS as the nucleation point for analysis software packages was emphasized as a major point! It was also discussed that the preparation of such nanostructured surfaces requires very specialized equipment and the prepared samples often cannot be removed from vacuum to protect their surfaces. This defined the requirement to carry out in-situ experiments, on the one hand, for performing real time polarized neutron reflectivity measurements during thin film coating processes (as requested by Peter Böni an in-situ coating facility would be required), but on the other hand also a site where complicated long-time experiments could be performed. In order to fulfil several complicated sample environment requirements at a single beamline, a beamline design was proposed where various quite complex sample environments (like an in-situ coating facility) would each be mounted on a dedicated movable platform, which could simply slide into position in the neutron beam at the beamline, but could also be operated independently if not used together with neutrons.

To foster the development of novel neutron scattering techniques, which are not specified today, an endstation is required which offers nothing but several beamports for test experimental setups (described as "a hole in the wall where neutrons come out").

After the discussion session, Coffee and a workshop photo was taken.



Workshop participants

After these, Dieter Lott (HZG), Sean Langridge (ISIS), Hartmut Zabel (RUB) and Clemens Ulrich (UNSW) presented various exemplary research studies on Chirality Effects, magnetic structures in 3 dimensions, non-collinear spinstructures and interface magnetism.

The final discussion round of the day, entitled "Technical Challenges for instrumentation/data analysis - what can and cannot be done today - where should we aim at ESS?" was chaired by Sean Langridge. At the beginning of the discussion round he summarized the main challenges on a slide, which were already

identified in previous discussion rounds and discussed in more detail, -- such as focussing (gain in flux for purely specular, homogeneous profile, directional moderators), backgrounds, spin-separation/recombination (Larmor labelling), detectors (dynamic range, spatial resolution), out-of-plane resolution, length scales, quality control (statistical & systematic errors), analysis (reduction/visualisation, theory, high perf. computing), Deuteration, software (reduction/analysis, pipeline development, data mining (big data)), sample environment (HT,T,P, shear, realistic surfaces (beyond Si)), dual colour measurements.

The most important point was again software development, where it was suggested to evaluate the existing software packages and to bundle the development at ESS for fast and easy-to-use fitting and simulation programs.

A dinner followed by discussions in smaller groups completed the day.

Fr. 26 Sept. 2014:

The instrumentation session saw the presentation of reflectometer designs: Jochen Stahn presented in his talk focusing optical elements in general and their possible applications at ESS (incl. a very brief description of the ESTIA reflectometer). Stefan Mattauch presented the design of another proposed reflectometer: VERITAS, which fostered a vivid discussion on the effective use of the ESS neutron pulses. As Charles Majkrzak could not attend the meeting, his scheduled talk on the coherence of neutrons on the observed scattering pattern was given by Brian Maranville per pro. After a brief coffee break, Hanna Wacklin concluded the presentation session with an overview of planned reflectometers and GISANS options at ESS.

The final discussion session of the workshop on "Science and functional requirements for future instruments - what should these be able to do?" chaired by Björgvin Hjörvarsson then essentially helped to summarize the workshop discussions:

The importance of a certain flexibility and of keeping space available to extend existing machines, whenever the need arises, was outlined. As a negative example, the limitations for extending flight-tubes given by a concrete wall behind SANS machines was mentioned and it was suggested that the experimental halls should be built significantly longer than required by the longest machines. However, it was also acknowledged that this increases the costs of the buildings. The importance of a GISANS option at a reflectometer was also discussed. It was agreed that these options should be available, but also that a dedicate (ToF-)GISANS setup should be built. The idea of sharing beam ports was also briefly mentioned.

Again, the importance of software packages for fitting specular and fitting (or at least simulating) off-specular patterns was emphasized and the sample environment requirements (e.g. cryostat, magnets, etc.) was briefly mentioned in terms of financing their realisation, which essentially concluded the workshop.

Summary and Recommendations:

The two major points which were repeatedly brought up during this workshop were the availability and design of scattering setups for collecting off-specular data from 2D (and in the future 3D) patterned samples, both in co-planar and GISANS geometry, and -- even more often -- the development of a suite of analysis, fitting and simulation software.

Important points and recommendations were:

- The designs of the two proposed reflectometers for liquids and solid systems at ESS with polarization option, having either a vertical or a horizontal scattering plane, were largely endorsed by the participants of the workshop and there was a strong motion towards that (polarized) GISANS should be an option at least for one of the reflectometers or at least that the design of the instruments should not exclude such an option from the beginning. It is, however, very well understood that an instrumental option would not be an optimized feature, but nevertheless, this option will be required. In any case, as off-specular signals tend to be weak, the reflectometers should be equipped with large area detectors that are shielded against background radiation as well as anyhow possible.

- The sample stages should be designed as to accept a large variety of sample environments, including low and high temperatures, low and high magnetic fields, MIEZE option, flow cells, high speed shear cells, etc. in order to allow the advantages of neutron reflectivity (NR) over XRR to be fully used (H-D contrast, other isotopic contrast, larger penetration depth, oxygen sensitivity, transmission of neutron beam through water bath for studying interfaces with water, transmission through thick silicon blocks, etc.).

- The trend in the future is also clearly towards more complex 2D and 3D patterned structures which might require to rethink the traditional classifications of (co-planar) off-specular and GISANS instruments and to investigate what scattering geometries might be needed instead: whilst reflectometers have high flux but large beam divergence perpendicular to the scattering plane, GISANS wins in the divergence, but at the cost of

sacrificing most of the flux. A combined, maybe tuneable, instrument which offers both, high flux and low perpendicular divergence, would be ideal.

- The participants demanded a user-friendly software package for fitting unpolarised and polarized specular neutron reflectivity data, which similar to e.g. FullProf finds the absolute minimum with high speed and provides a profile of the scattering length density. For off-specular diffuse scattering a software package should be provided that is capable of at least simulating (if not fitting) the off-specular diffuse intensity in a DWBA approach. As available software packages have been programmed by users in a more or less semi-professional way, which will not meet the needs of the future requirements in this field, it was highly recommended that professional programmers and scientists, working hand-in-hand, will be involved in these efforts. In this context, a collaboration with the synchrotron community should help to foster the developments.