

## Report of the reflectometry STAP meeting 24-25.09.19

STAP committee: Frank Heinrich, Robert Jacobs, Kelly Morrison, Frank Schreiber and Mike Fitzsimmons (chair) (Peter Müller-Buschbaum was unavailable)

ESTIA instrument team representative: Artur Glavic

FREIA instrument team representative: Thomas Arnold, Jon Elmer

ESS: Ken Andersen, Andreas Schreyer, Wojciech Potrzebowski, Francesco Piscitelli, Richard Hall-Wilton, Oliver Löhmann

### Actions items:

Item	Recommend action	Progress
1 (Estia)	Further tests, analysis and report on the multiblade detector.	Work in progress.
2 (Estia)	Report on comprehensive background calculation.	Work in progress.
3 (Freia)	McStas simulations to produce R(Q).	Work in progress. WFM optimization progressing (if not completed?). Arnold has a plan for data reduction and analysis.
4 (Freia)	Question 1: What is the worst angular resolution that is likely to be useful? What is the smallest sample footprint for which this resolution is required?	$\Delta\theta/\theta \sim 10\%$ for 4 cm <sup>2</sup> samples. Rationale: Sacrifice resolution for intensity required for kinetic experiments which will usually utilize fairly large samples.
5 (Freia)	Question 2: Where should the polarizer be placed?	Either in front of the upstream collimation slits or after the sample on the detector arm. Rationale: ½-polarization beam option for magnetic reference layer work.
6 (Freia)	Question 3: What is the minimum Q required?	$Q_{min} \leq 0.005 \text{ \AA}^{-1}$ (0.004 $\text{\AA}^{-1}$ would be better.) Rationale: Calculation performed for contrast across a water/alcohol interface.

7(Software)	Beyond what is listed in the background material, provide a detailed inventory of what BornAgain <i>does now</i> , and what BornAgain <i>will do</i> in the future as a consequence of the ESS software investment. Fitting specular reflectivity should be high on the priority list for development, testing and available well before instruments become operational.	Per Wojciech, he will provide.
8 (STAP)	Provide guidance to software group on what BornAgain needs to do.	Focus subject for future STAP meeting.

This year's reflectometry STAP meeting partially overlapped with the SANS STAP. The overlap provided the opportunity for the STAP's to hear a plenary presentation updating the status of the ESS project. We found this change useful; however, if an intent is to compare notes between the committees, then some time should be explicitly dedicated for this purpose. In the future, the reports of the two STAPs should be shared between the committees.

### ***Detector progress***

The STAP is very impressed with the quality of the data collected by the new multi-blade detector technology, and the STAP is equally impressed with the work of the development team led by Dr. Francesco Piscitelli who exudes professionalism and passion for the project. The STAP welcomes and appreciates the engagement of Dr. Richard Hall-Wilton during our meeting. The STAP learned a lot from the presentation—particularly about the advantages and disadvantages of multi-blade detectors compared to  $^3\text{He}$  detectors.

- The multi-blade detector has  $\sim 2/3$  the efficiency of a  $^3\text{He}$  detector for  $\lambda < 6 \text{ \AA}$  and comparable efficiency for  $\lambda > 6 \text{ \AA}$ .
- Due to the low recoil of Ar compared to He for collisions with fast neutrons, the multi-blade detectors have 10-100x lower sensitivity (which is good) to fast neutrons compared to  $^3\text{He}$  detectors.
- Francesco quantified the influence of the Al window thickness on background. Thick Al windows—such as required for high pressure  $^3\text{He}$  detectors—cause higher background than thin windows. Because multi-blade detectors operate at atmospheric pressure, only a thin window is required to isolate the Ar-quench gas. This means compared to  $^3\text{He}$  detectors the Al window produces less background for multi-blade detectors. However, owing to the thin window and the 1 bar pressure of the Ar gas, multi-blade detectors are sensitive to variations of atmospheric pressure at the level of a couple percent. This sensitivity is undesirable but can be either actively compensated or corrected via software (the latter is probably a more reliable solution).

- Multi-blade detectors use two crossed layers of wires and coincidence detection to achieve spatial sensitivity. Coincidence further reduces sensitivity to background from random sources, e.g.,  $\gamma$ -rays.

We suggest ORNL may be interested in the multi-blade detector and encourage K. Andersen to arrange a demonstration.

### ***Freia Progress***

Dr. Thomas Arnold (Freia instrument scientist), Mr. Jon Elmer, and Dr. Oliver Löhmann presented progress on the Freia project. The STAP appreciates Thomas having brought questions to the STAP—these are answered in the table above. The two most important matters involved Rainbows (energy measurement using prisms) and testing of the wavelength frame multiplication (WFM) technique.

### ***Rainbows***

Prior to Thomas joining the Freia team, an earlier STAP regarded Rainbows as a backup plan should the preferred solution to use WFM choppers fail (owing to technical difficulties in rotating large diameter chopper blades). However, mechanical testing of the WFM choppers was very promising, so in 12/2018 (see our STAP report) the STAP recommended against pursuing Rainbows (as an alternative to WFM). During the 9/2019 meeting, Thomas alerted the STAP to the possibility that Rainbows might be able to yield a 2-fold improvement in performance for  $\Delta Q/Q \sim (4 \pm 1)\%$ , provided the spatial resolution of the multi-blade detectors could be reduced from 0.55 mm to 0.3 mm. This further challenge to the detector project involves significant R&D effort of bandwidth-limited staff, and either requires a composite 1D/2D design or sacrifice of 2D capability altogether (and thus GISANS). The STAP was not compelled that these sacrifices are worth the improved performance in a small fraction of the resolution range of Freia. The STAP recommends Rainbows not be included in Freia. The STAP commends Thomas for his initiative with regards to exploring this option prior to commitment of the detector design.

### ***Testing the WFM concept***

Dr. Oliver Löhmann reported testing of the WFM concept using the V20 instrument at HZB Berlin. The WFM concept enables Freia to achieve the best possible resolution while taking advantage of the long proton pulse to maximize the intensity of the incident neutron beam. This involves time focusing of the neutron beam at the position of the WFM chopper. As such, each short neutron pulse that passes through the chopper is time shifted relative to the former. The V20 experiment successfully demonstrated, for the first time, an algorithm that effectively time-splices the incident beam spectrum, i.e., removes the gaps in time-of-flight observed in the raw data. The team used the time-shifted spectrum measured for the direct beam to normalize reflectivity data collected from a Si substrate and a demagnetized magnetic superlattice. The results appear promising (particularly to the untrained eye). Additional

analysis is required to properly account for background and to understand the origin of differences of the reflectivities taken using V20 and V6 (a purpose-built reflectometer) of the same sample.

### *Estia Progress*

Dr. Artur Glavic presented progress of the Estia project. Progress is on track to allow hot-commissioning of the instrument when first neutrons become available. The STAP compliments Artur on the attention he pays to budget and for creative solutions to mitigate disparity between cost estimates obtained for TG2 (in 2016) with those actually provided in 2019. Hopefully, lessons learned from Estia's experience will aid Freia in the future.

Artur reported on concepts to polarize the neutron beam and to mitigate frame overlap using components located at the middle focus position. Artur argued that the instrument can achieve the original specifications for Estia after realizing that the specifications do not need to be satisfied simultaneously (rather they are specifications dictated from a range of experimental conditions that are not necessary at the same time). Artur proposed a solution involving use of one or two polarizing supermirrors of different capabilities that could be remotely inserted at the middle focus position. One of these polarizers will serve as a frame overlap mirror. For unpolarized beam experiments a specially built frame overlap mirror will be (remotely) inserted.

Artur performed simulations of the polarization performance for his solutions, which suggest the solutions will perform adequately.

The committee cautions that on account the mirrors will require tiling smaller mirrors together, small gaps between the tiles may degrade performance. For example, a portion of the neutron beam may only interact with one of the two coatings, or none at all. For the case of frame overlap rejection, the neutron beam has only one chance to interact with the Si substrate, so a gap between the tiles will degrade performance. Gaps between the tiles were not considered in the simulations. Simulations should be performed to establish a fabrication metric for the product, e.g., How large a gap can be tolerated to meet the polarization and frame overlap rejection criteria?

Fitzsimmons reported the presence of very small angle scattering of the polarized neutron beam (that was spin flip) resulting in satellite reflections about the main beam from Swiss Neutronic mirrors. Fitzsimmons sent information to Glavic and Andersen.

### *Software*

Due to unfortunate scheduling of the reflectometry, SANS and DMSC STAPs at the same time, engagement with DMSC was curtailed. Fortunately, Dr. Wojciech Potrzebowski provided an update on the BornAgain (BA) project. The reflectometry STAP is concerned that as BA was originally intended for GISAS that the project receive adequate resources to ensure BA

performs analysis of specular reflectometry that is at least as functional as the best existing packages (e.g., Genx, Motofit, Ref1d). Because the specular reflectometry community dwarfs the GISAS community, and BA is envisaged to be “the supported package” for specular reflectometry analysis at ESS, the adapted package must be attractive to an entrenched community, i.e., a community that is already wedded to existing and proven options. The STAP recommends:

- The next meeting in Lund be primarily focused on all matters related to data *acquisition* and *analysis* for ESTIA/FREIA.
- Invite a representative from Jülich to the meeting.
- Arrange a live demonstration of BA for specular reflectometry to the STAP.
- Engagement with specular reflectometry users to ensure functionality.
- Development of a strategic plan to socialize and educate the community on BA for specular reflectometry well before 1<sup>st</sup> users of ESTIA arrive.

The STAP is willing to invest time to download BA, to test it, and to read documentation prior to the next face-to-face meeting.

Tom Arnold will forward details of ISIS based reflectometry software meeting on 24/25 October to K. Morrison and R. Jacobs, and agreed to ask the organizers to contact them to allow registration at the event.

The STAP appreciates and commends DMSC’s leadership in organizing a workshop in Copenhagen (9/19) on machine learning and x-ray/neutron scattering. Fitzsimmons and Heinrich from the STAP attended this meeting.