SESANS Standards Working Group Meeting (20 January 2023)

Attendees

Wim Bouwman (WGB), Rob Dalgliesh (RMD), Henrich Frielinghaus (HF), Fankang Li (FL), Roger Pynn (RP), Gregory Smith (GNS)

Update since last meeting

GNS welcomed everyone to the meeting. No progress had been made on the SmortPor membranes. GNS acknowledged SRP for a great job representing the group at the recent canSAS-XII meeting in Brazil and passed questions from the session to the group (about where data would be stored and about future file formats).

Facility updates

ISIS (RMD)

The Larmor system is now much more stable and can perform reliable SESANS measurements. It was recalibrated using of RP's gratings, and a new one had been purchased (5 μm deep gratings, area 10x20 mm, either 1 μm or 500 nm periods).

TU Delft (WGB)

The instrument is now running again after the long shut down, although it is now in the reactor hall. It has the same performance as before. Even after the cold source is installed, this instrument will remain in the reactor hall, and there is the possibility of commissioning a dedicated SEMSANS instrument on a beam port on the cold source.

ORNL (FL)

Test measurements (PMMA in d-decane, flexible graphite sheets, alumina membranes) had been performed on several beamlines at HFIR (two test beamlines at 4.2 and 5.5 Å). Data were reproducible week-to-week. Additionally, tests were made on the Q coverage (by changing apertures, made sense) and sample rotation (signal changed dramatically, still trying to comprehend). They have 24 days planned operation in March 2023, with no plans after that (need to get time on test beamline).

Cross-instrument measurements

FL's experience running the membranes sparked a discussion about their structure in SANS/SAXS as well. This had been seen by others: RMD on Larmor SANS, WGB on Grenoble SAXS, and HF on NIST SANS. This asymmetric 2D scattering suggested the pores were not aligned to the beam. This could be tested by running samples at different rotations with respect to the beam; this prompted general discussion about the importance of encoding direction with aligned samples.

The difficultly in understanding the SANS/SAXS of membranes (let alone SESANS) suggests that they are not candidates for calibration standards. Graphite foils studied at ORNL were invariant; they are perhaps not calibration standards but would be good for reproducibility. It was agreed that this should be shared between facilities for to compare data.

FL updated group with the plan of colleague (Wei-Ren Chen, ORNL USANS) to include a parallel session about long length scale scattering (USANS and SESANS) at upcoming SAS2024 meeting. The group discussed how to communicate SESANS data to those

familiar with reciprocal-space scattering. (Should SESANS data be turned back into *Q*-space? But if you have a real-space technique, why go back to reciprocal space? Should we not meet users where they are?) RP raised the matter of multiple scattering. SANS tends to use weakly scattering samples to avoid multiple scattering, whereas SESANS gets better data with multiple scattering. This is something that will need to be revisited.

Data format

Inspired by a question from the canSAS-XII presentation, the group discussed the current and future of SESANS data and analysis. RMD felt that the file format was fine (contained all required information) but that it was not being used correctly. A new format ("NXSESANS") might be required when 2D SESANS is achieved, but WGB felt that would be a non-standard thing so was not high priority. The most important development for data analysis would be to get funding for programmes to work on analysis software, such as SasView.

Actions

- **RMD** to distribute XRnanotech details to the group.
- **FL** to distribute details of flexible graphite to the group and samples to other facilities (ISIS and TU Delft).
- **All** to consider what would need to done with SESANS technique to enable its promotion at SAS2024.
- **All** to consider funding opportunities to work on software for SESANS data analysis (SasView).