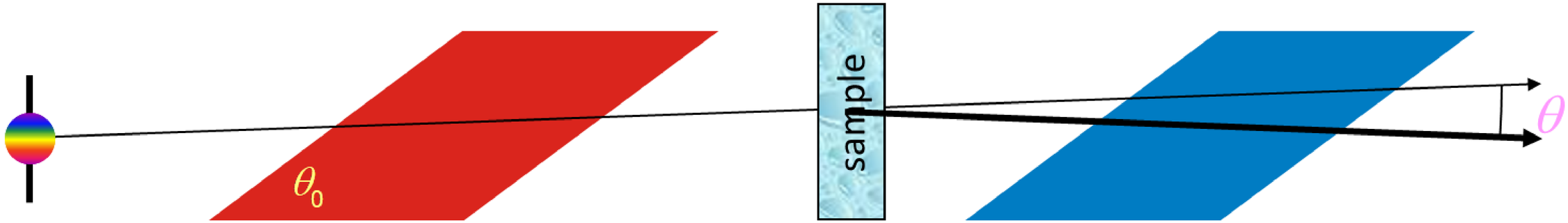


SESANS Reproducibility Working Group

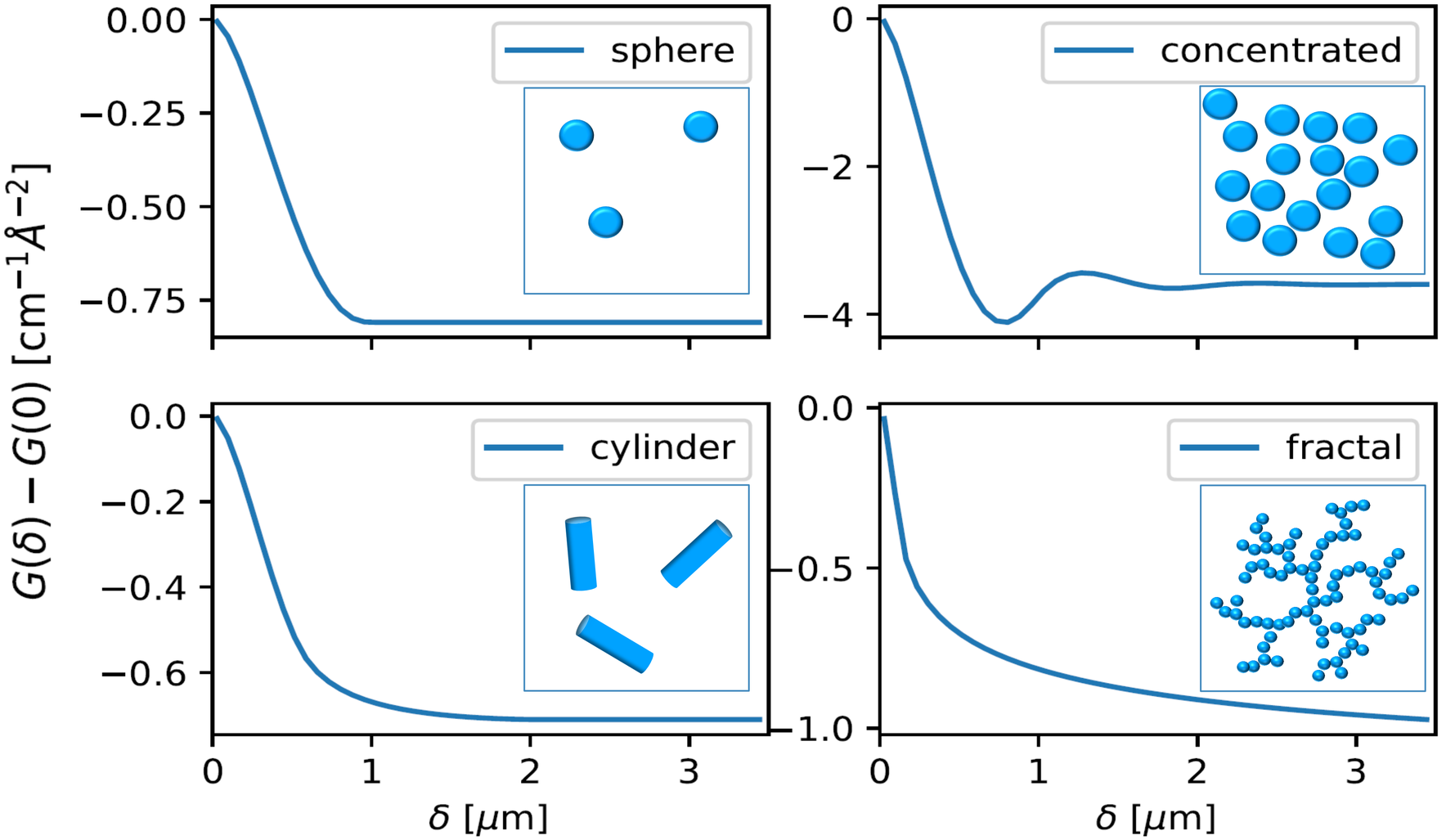
Update and Activities

canSAS-XIV at SAS2024 (Taipei)—3 November 2024

Gregory Smith (ISIS)—Working Group chair
Wim Bouwman (TU Delft)—Presenter

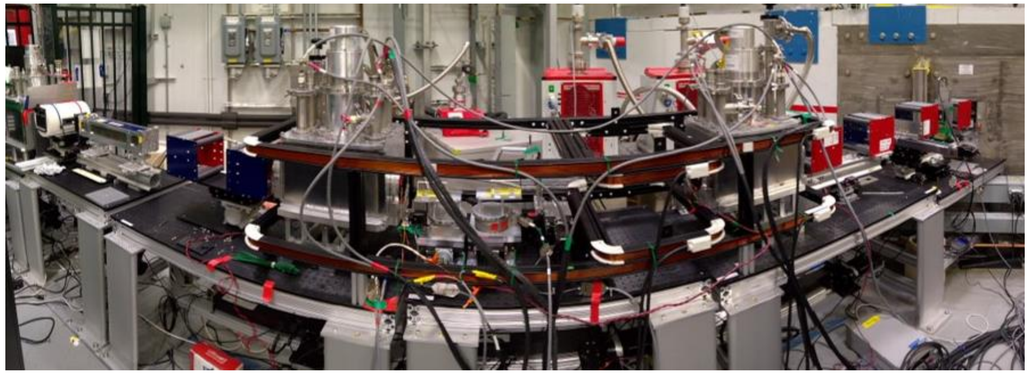
Spin-echo small-angle neutron scattering

SESANS

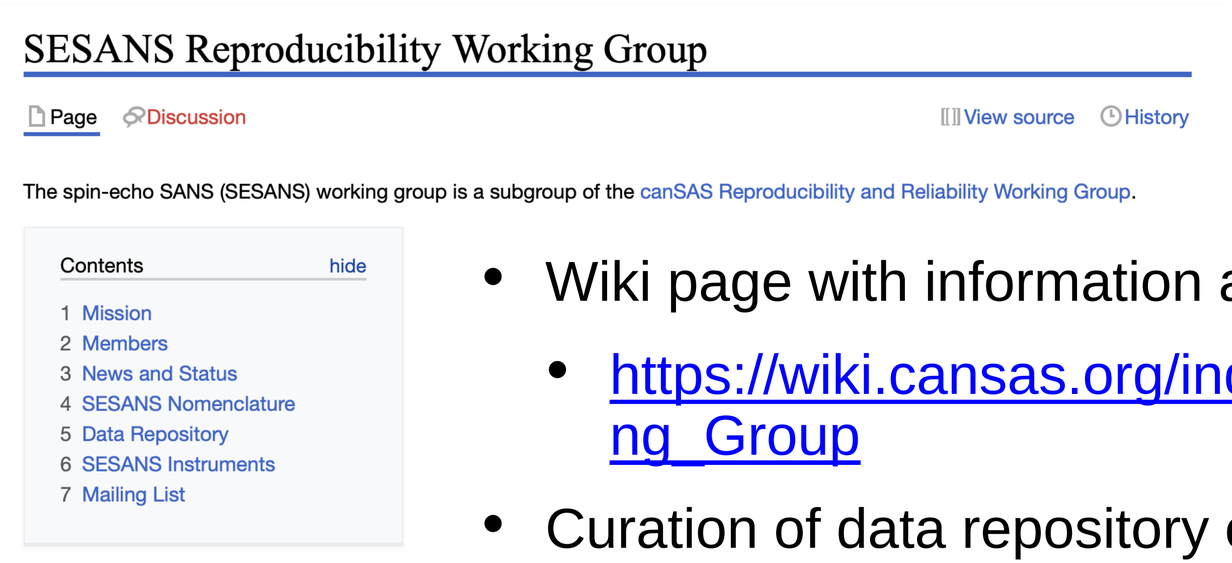


Working Group members

- Wim Bouwman (TU Delft)
- Robert Dalgliesh (ISIS Neutron and Muon Source)
- Henrich Frielinghaus (Jülich Centre for Neutron Science, MLZ)
- Fankang Li (Oak Ridge National Laboratory)
- Andrew Parnell (The University of Sheffield)
- Steven Parnell (ISIS Neutron and Muon Source)
- Roger Pynn (Indiana University Bloomington)
- Gregory Smith (Chair, ISIS Neutron and Muon Source)



Group Activities



SESANS Reproducibility Working Group

Page Discussion View source History

The spin-echo SANS (SESANS) working group is a subgroup of the canSAS Reproducibility and Reliability Working Group.

Contents hide

1 Mission
2 Members
3 News and Status
4 SESANS Nomenclature
5 Data Repository
6 SESANS Instruments
7 Mailing List

- Wiki page with information about SESANS and links to instruments
  - https://wiki.cansas.org/index.php?title=SESANS_Reproducibility_Working_Group
- Curation of data repository of possible SESANS standards
  - https://zenodo.org/communities/sesans_reproducibility_working_group/
- Mailing list of SESANS-related updates
  - https://www.jiscmail.ac.uk/cgi-bin/webadmin?SUBED1=SESANS-WORKING-GROUP&A=1

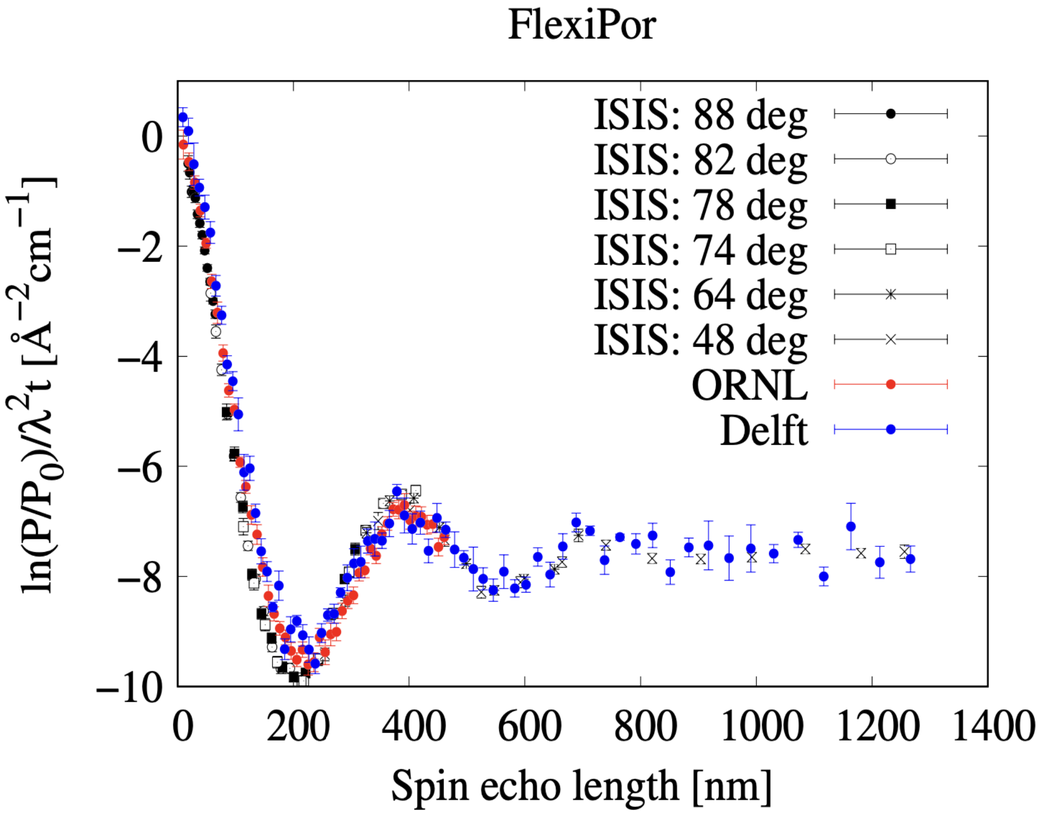
Agreed nomenclature for SESANS data

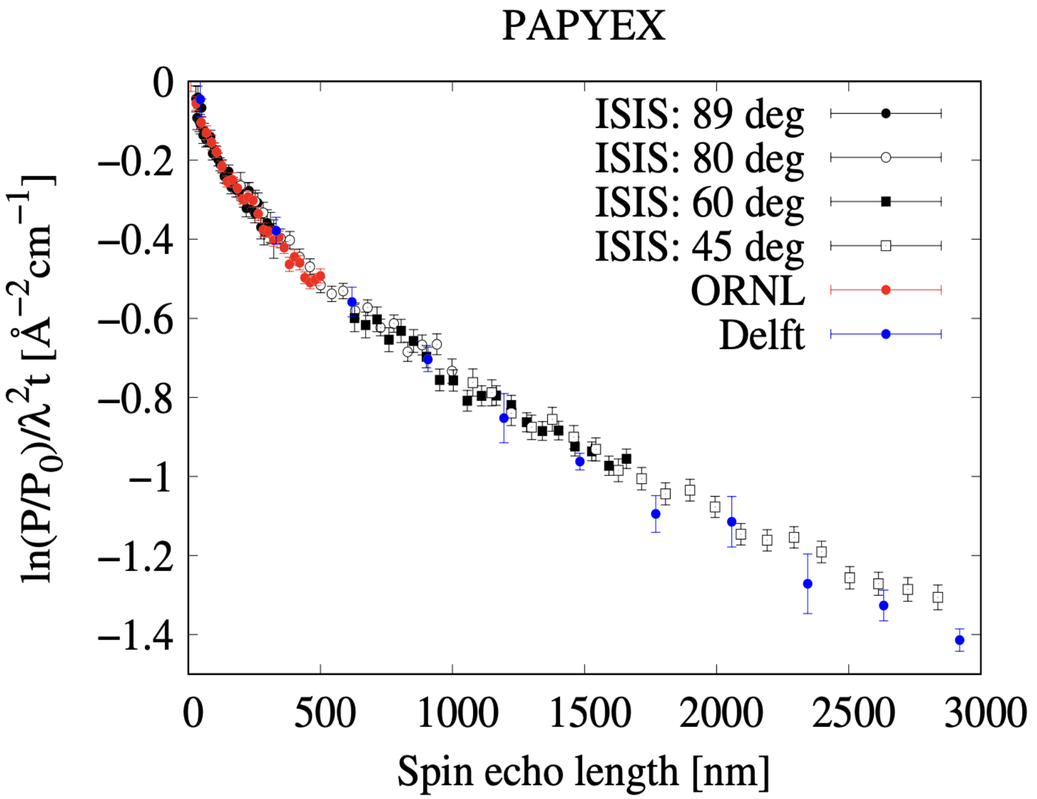
Statement available on CanSAS wiki

- **SESANS data function of "spin-echo length" δ.**
  No preferred unit, (μm, nm, or Å) whatever suits natural length scale sample.
- **SESANS data measured "normalized scattering correlation function".**
  Normalization measured polarization sample (P) with polarization reference (P_0).
  Combined to recommended presentation of SESANS data, the natural logarithm of P/P_0 divided by sample thickness (t) and the square of the neutron wavelength (λ^2), for brevity $\ln(P/P_0)/(t*\lambda^2)$.
  Instrument and wavelength independent data.
  No recommended variable for the normalized scattering correlation function.
  We recommend unit (cm^{-1} $Å^{-2}$), natural units sample thickness (cm) and for neutron wavelength (Å).

Cross-calibration of SESANS instruments

- Porous alumina membrane flexible graphite: ORNL, TU Delft, and ISIS (Larmor)





Many thanks to Fumiaki Funama (ORNL) for collating data

SESANS file format

- Text-based SES format with header and four-column data.
- Improve header with unequivocal identification of data and facility.
- What to include in future Nexus based file format.

88214_sesans_tcorr.ses

```
FileFormatVersion       1.0
DataFileTitle           {ORNL FlexiPor -88deg 1MHz Scruffy}_SESANS
Sample                  88214
Thickness               0.060000
Thickness_unit          mm
Theta_zmax              0.10000000000000001
Theta_zmax_unit         radians
Theta_ymax              0.10000000000000001
Theta_ymax_unit         radians
Orientation             Z
SpinEchoLength_unit     A
Depolarisation_unit     A-2 cm-1
Wavelength_unit         A
Echo_constant           26.494816936180609

BEGIN_DATA
SpinEchoLength Depolarisation Depolarisation_error Wavelength
179.105 -0.49888 0.142202 2.6
207.719 -0.662651 0.118221 2.8
238.453 -1.01359 0.102436 3
271.307 -1.01216 0.092399 3.2
306.28 -1.12373 0.0850063 3.4
343.373 -1.41995 0.0790347 3.6
382.585 -1.58498 0.0738817 3.8
423.917 -1.79894 0.0683251 4
467.369 -2.07709 0.0623868 4.2
512.94 -2.39655 0.0591027 4.4
560.63 -2.64254 0.056531 4.6
610.441 -2.99566 0.0548285 4.8
649.189 -3.23433 0.076687 4.95
```

Data corrections

- Neutron wavelength and finite detector size impact experimentally determined data.
- Simple corrections using transmission.
- Desire: understand corrections. Reproducibility measurements different sources (mono vs ToF, different λ).

SCIENTIFIC REPORTS

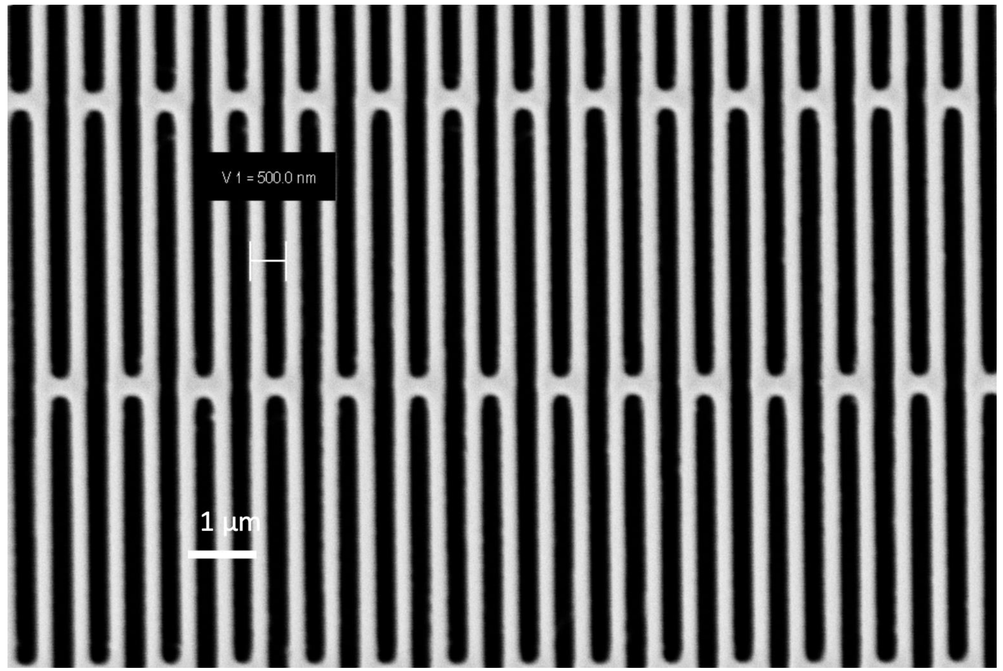
OPEN

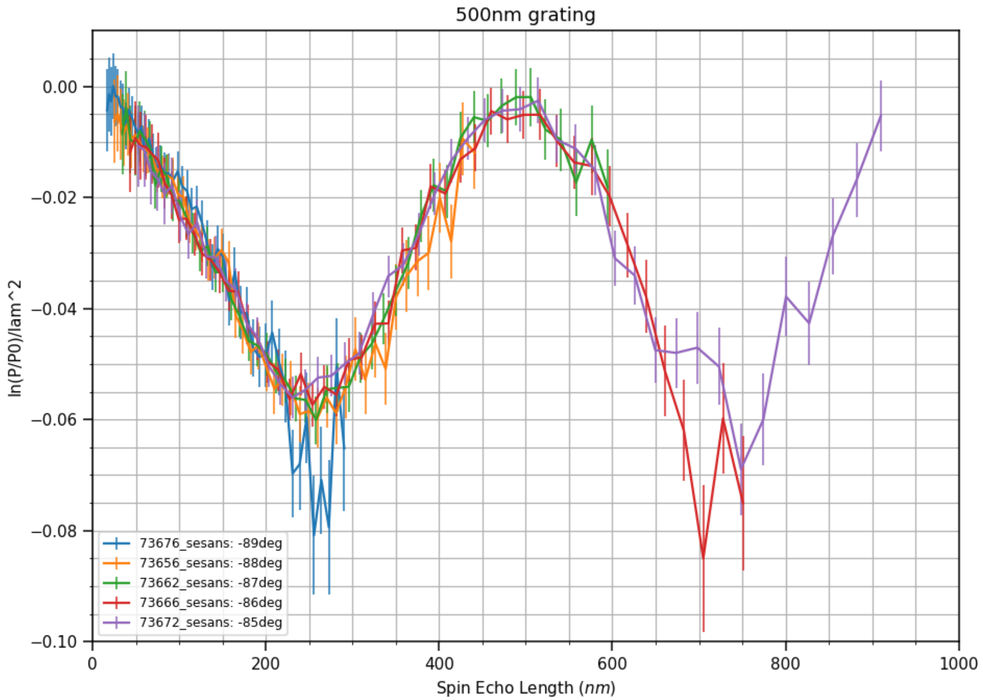
Data Correction of Intensity Modulated Small Angle Scattering

Fankang Li[1], Steven R. Parnell[2], Robert Dalgliesh[3], Adam Washington[3], Jeroen Plomp[2] & Roger Pynn[1,4]

Standard samples for calibration

- Cross-calibration data for understanding SESANS measurements to get comparable data from different facilities.
- Currently, gratings with well-defined spacings (see below 0.5 µm).
- Need better options calibration standards (spin-echo length and depolarization). Ideally primary standards on length scales from ~40 nm to ~40 µm.





SESANS reproducibility working group

- Communication platform
- Nomenclature and symbols
- Cross calibration
- Standard file format

- Data corrections
- Standard samples