

# SESANS Reproducibility Working Group

**Update and Activities**

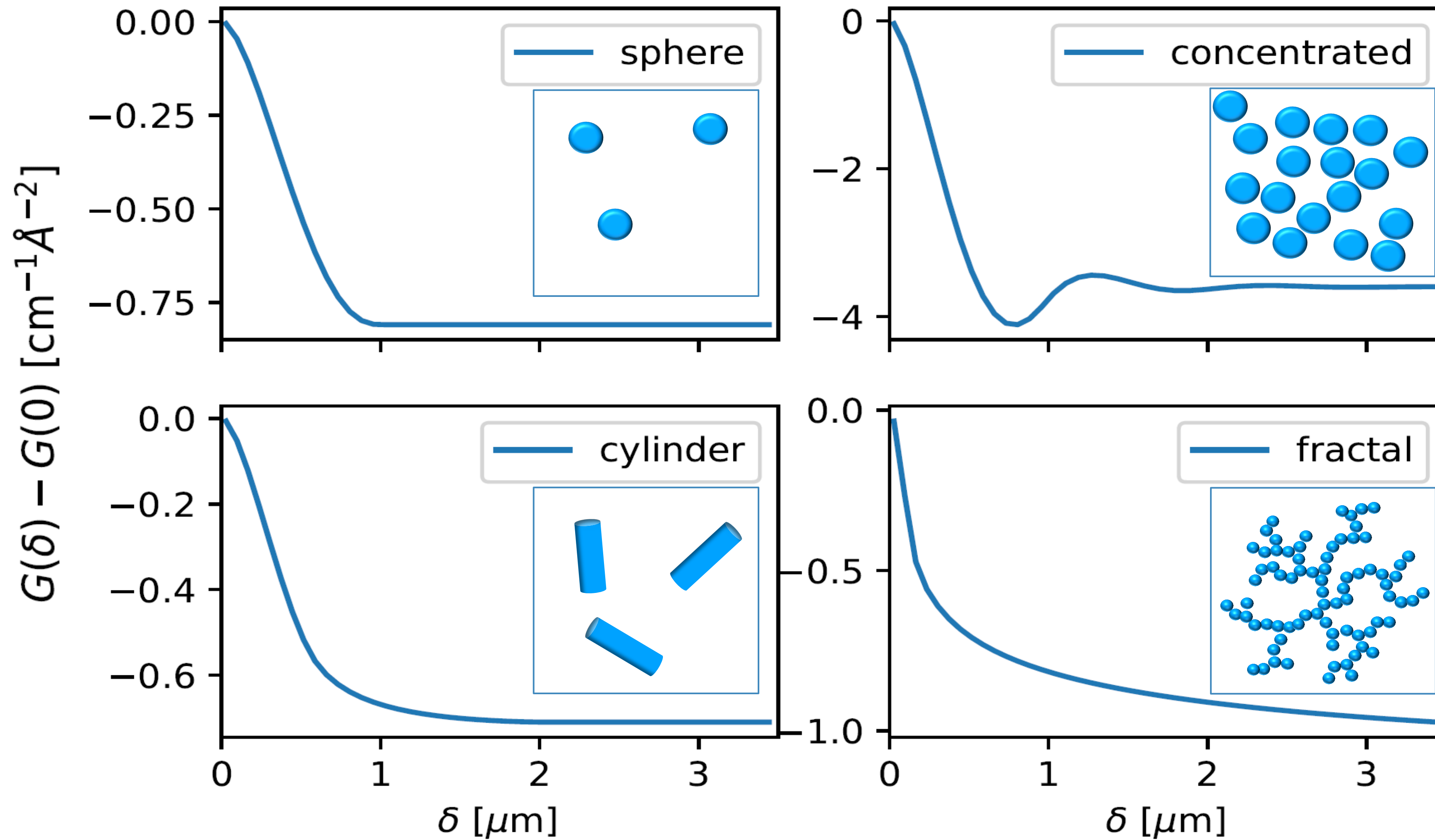
canSAS-XIV at SAS2024 (Taipei)—3 November 2024

**Gregory Smith (ISIS)—Working Group chair**

**Wim Bouwman (TU Delft)—Presenter**

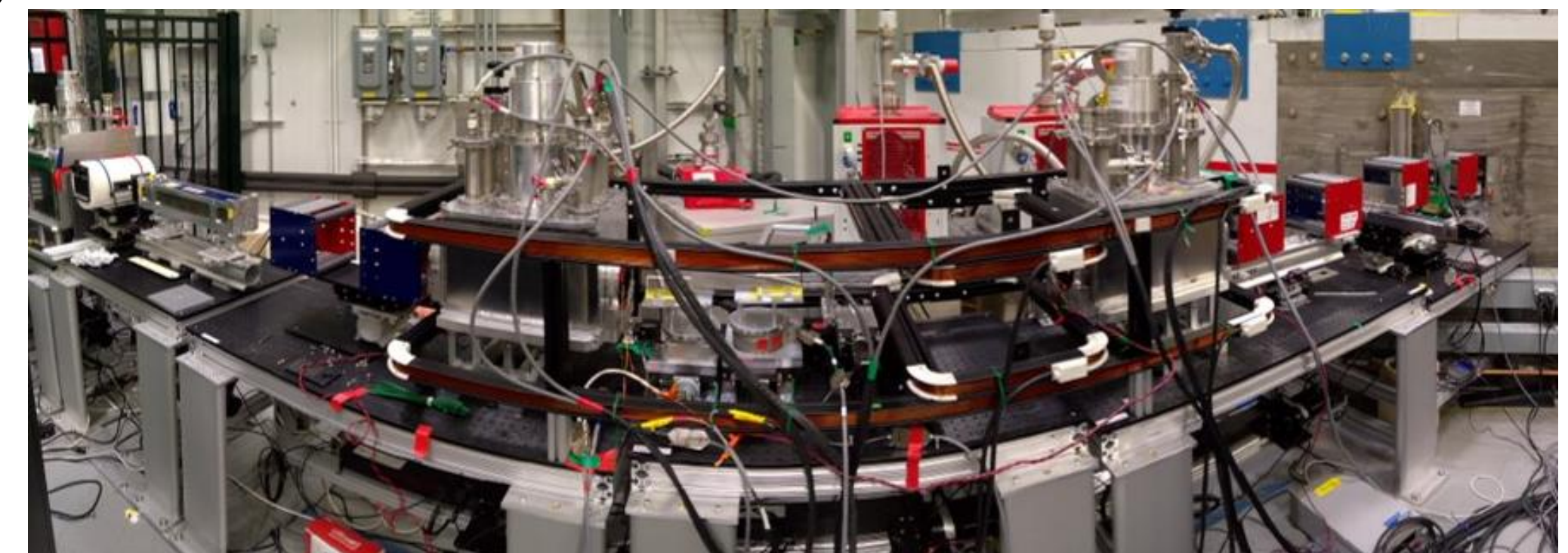
# Spin-echo small-angle neutron scattering

## SESANS



# Working Group members

- Wim Bouwman (TU Delft)
- Robert Dalglish (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

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

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- Wiki page with information about SESANS and links to instruments
  - [https://wiki.cansas.org/index.php?title=SESANS\\_Reproducibility\\_Working\\_Group](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/](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>

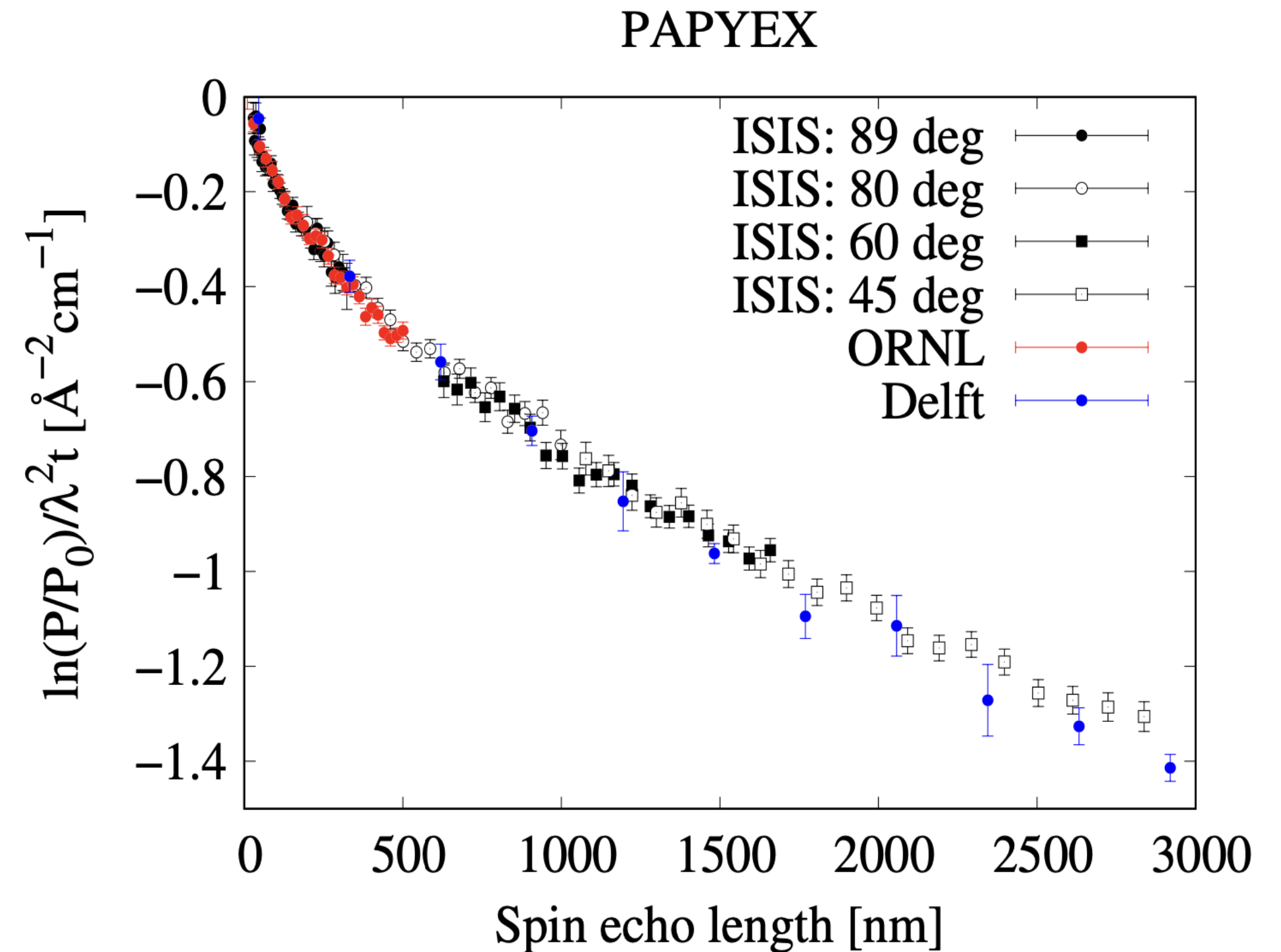
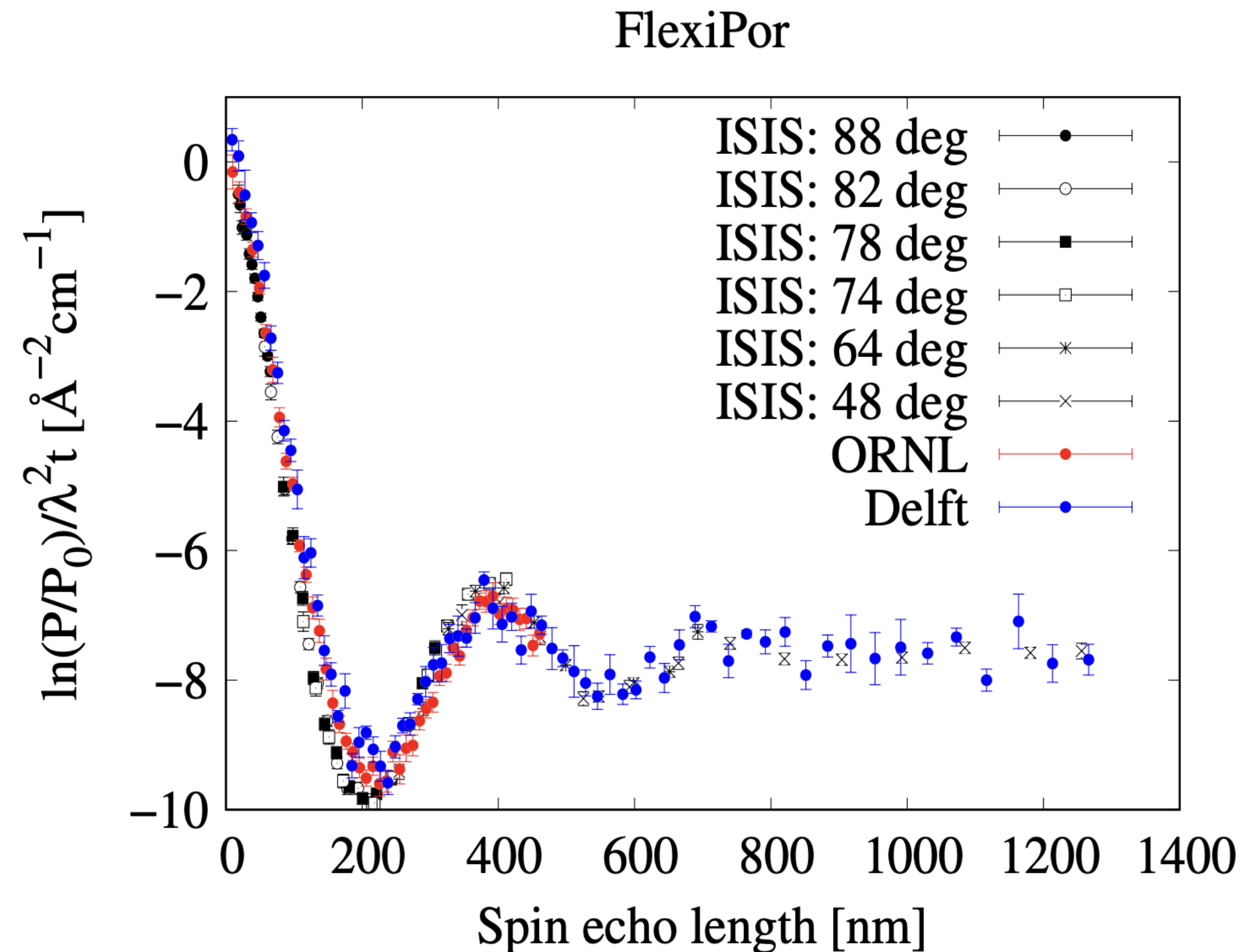
# Agreed nomenclature for SESANS data

Statement available on CanSAS wiki

- **SESANS data function of "spin-echo length"  $\delta$ .**  
No preferred unit, ( $\mu\text{m}$ ,  $\text{nm}$ , or  $\text{\AA}$ ) whatever suits natural length scale sample.
- **SESANS data measured "normalized scattering correlation function".**  
Normalization measured polarization sample ( $P$ ) with polarization reference ( $P_0$ ).  
 **$\ln(P/P_0)/(t*\lambda^2)$ .**  
Instrument and wavelength independent data.  
No recommended variable for the normalized scattering correlation function.  
We recommend unit ( $\text{cm}^{-1} \text{\AA}^{-2}$ ), natural units sample thickness ( $\text{cm}$ ) and for neutron wavelength ( $\text{\AA}$ ).

# Cross-calibration of SESANS instruments

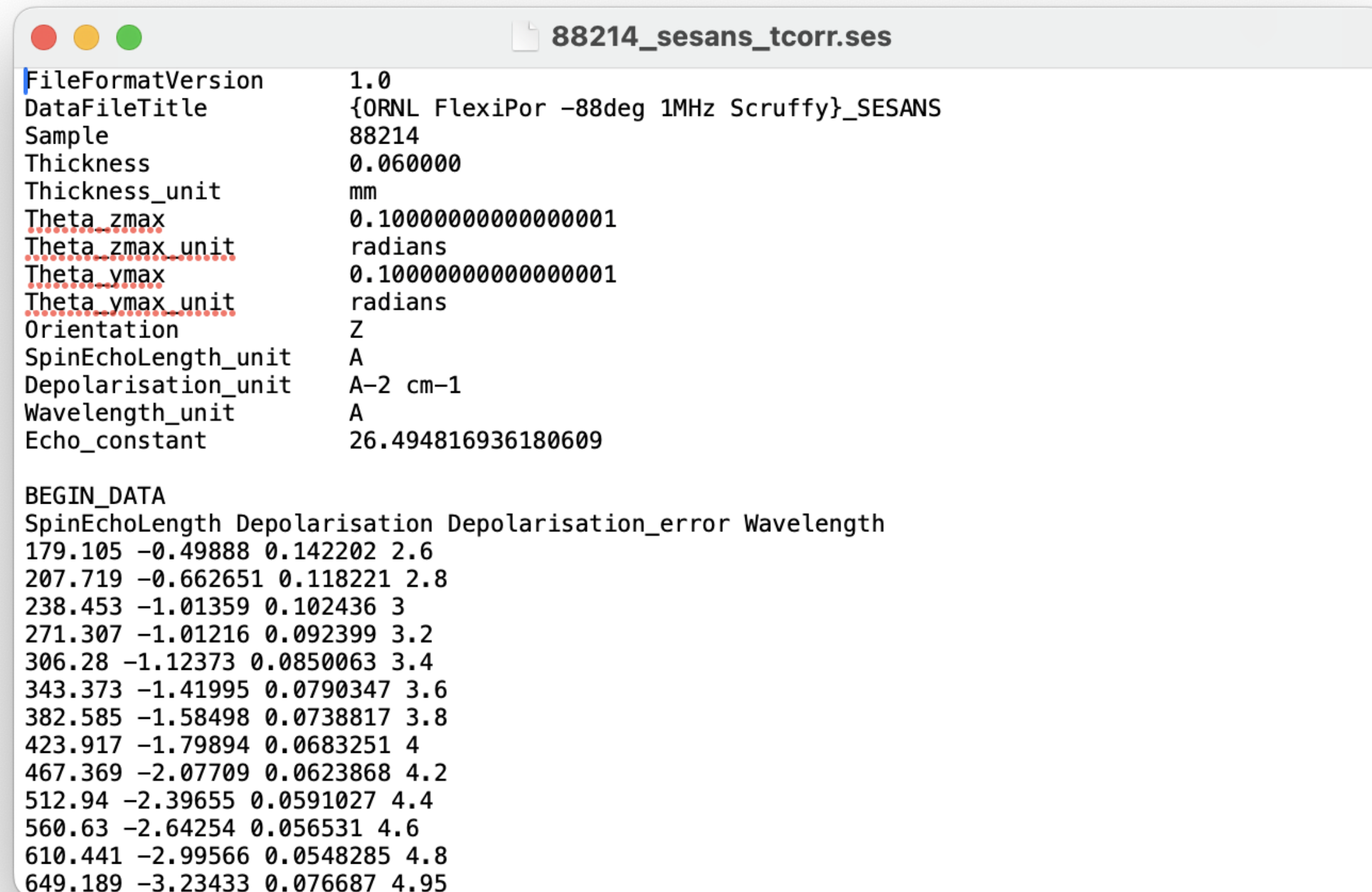
- Porous alumina membrane flexible graphite: ORNL, TU Delft, and ISIS (Larmor)



*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             0.100000000000000001
Theta_zmax_unit       radians
Theta_ymax             0.100000000000000001
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  $\lambda$ ).

SCIENTIFIC REPORTS

OPEN

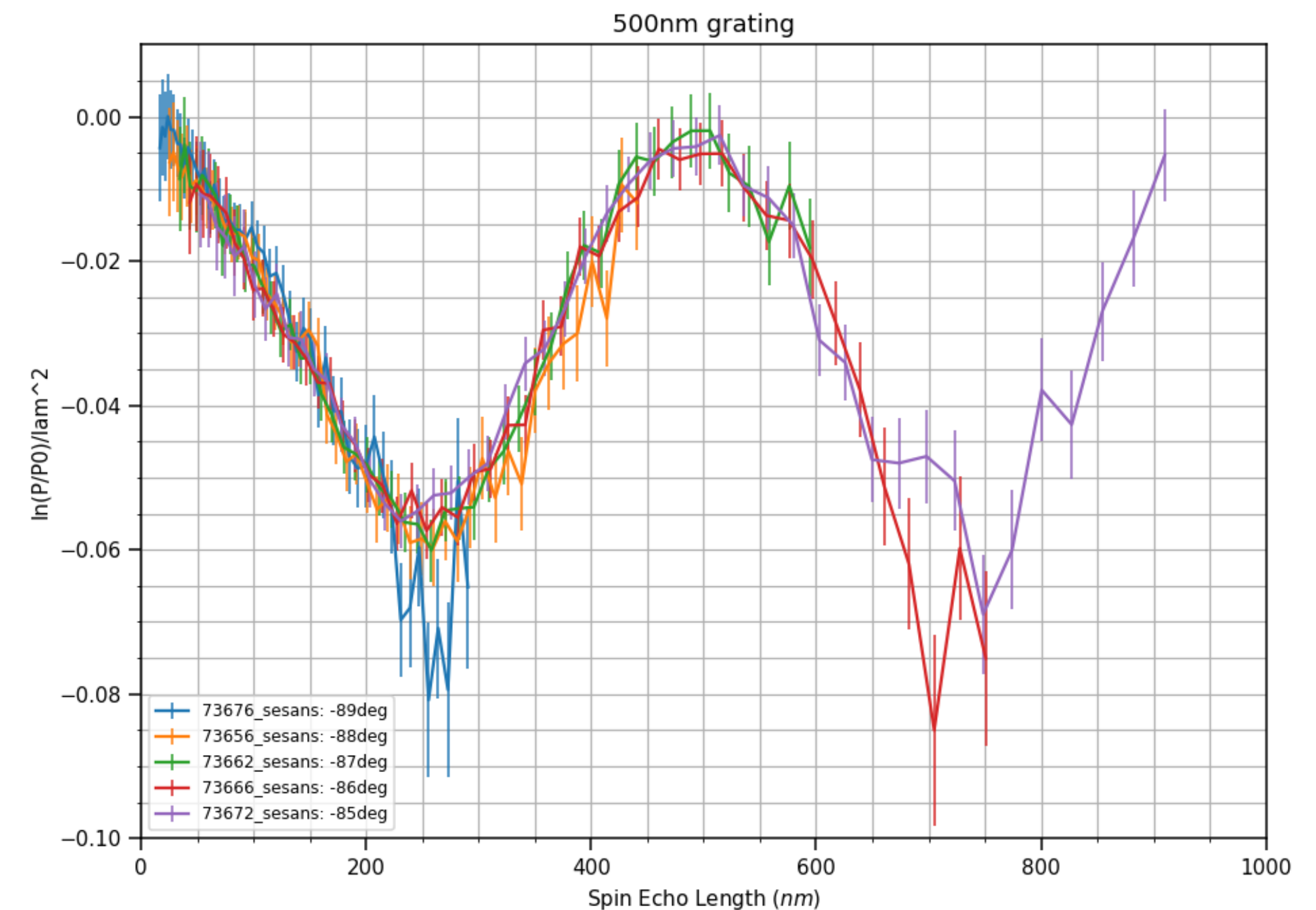
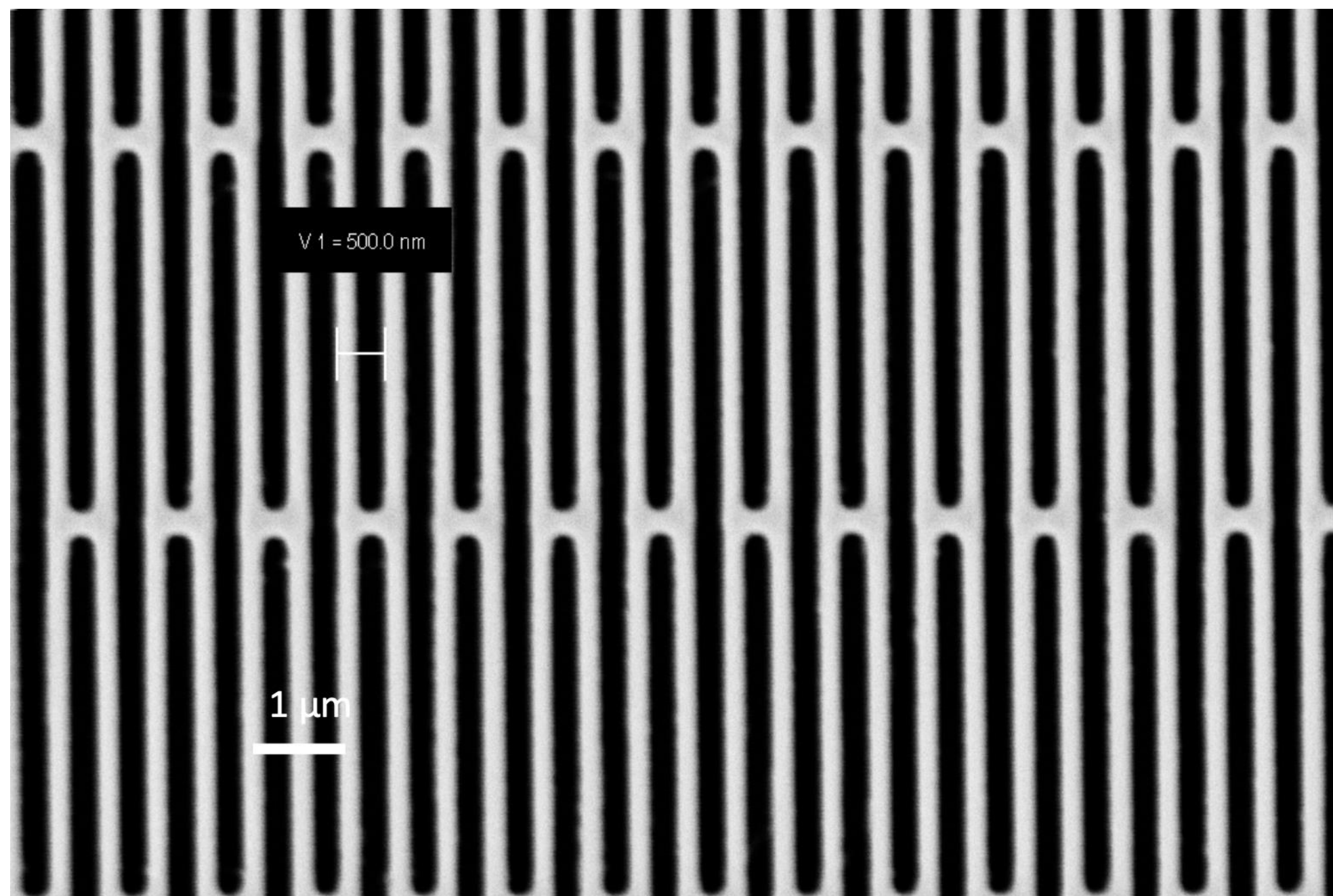
## Data Correction of Intensity Modulated Small Angle Scattering

Fankang Li <sup>1</sup>, Steven R. Parnell<sup>2</sup>, Robert Dalglish <sup>3</sup>, Adam Washington<sup>3</sup>, Jeroen Plomp<sup>2</sup> & Roger Pynn<sup>1,4</sup>



# 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  $\mu\text{m}$ ).
- Need better options calibration standards (spin-echo length and depolarization). Ideally primary standards on length scales from  $\sim 40$  nm to  $\sim 40$   $\mu\text{m}$ .



# SESANS reproducibility working group

- Communication platform
- Nomenclature and symbols
- Cross calibration
- Standard file format
  
- Data corrections
- Standard samples