SNS-NSE

The Neutron Spin
Echo Spectrometer @ SNS

Laura-Roxana Stingaciu

Large Scale Structures Group

Beamline Review Checklist

1. SNS-NSE beam line overview
2. Scientific Mission and Impact
3. General User Program
4. Beamline productivity
5. Software, sample environment and ancillary equipment
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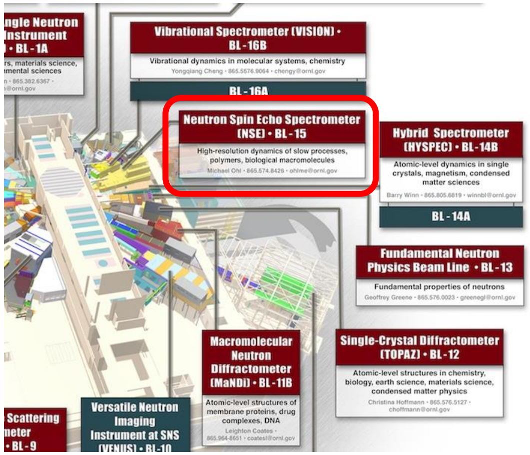
8. Summary & Vision

SNS-NSE, BL15 Overview

- Ultrahigh resolution spectrometer for characterizing slow dynamics of soft condensed matter @ nanoscopic and mesoscopic scale
- Detects neutron velocity changes < 10^{-5}
- SNS-NSE was built and operated by *FZJ* until April 2020, currently in transition to *ORNL*
- The first NSE spectrometer at a pulsating source
- The first NSE spectroscopic design based on superconducting technology
- The only NSE spectrometer with magnetic shielding



SNS-NSE Instrument Specifications

main precession	SC coils, actively shielded
field integral	J = 0.56 Tm
moderator	cold-coupled hydrogen
neutron guide h x b	Ni coated 4 x 8 cm^2
wavelength selection	system of 4 choppers
wavelength frame	2Å < λ < 14Å BW 3.6Å – 2.4Å
declination angle	3.5°
max. scattering angle	29/42/56/79° conf. dependent
sample size	30 x 30 mm^2
analyzer	Supermirrors
temperature range	TFS: -80+375C Cryo: 5K : 650K

moderator - sample distance: → 18 m, 21 m, 24 m, 27 m sample - detector distance: → 4 m	30x30 cm^2 ^{3}He DENEX detector → 32x32 pixels TOF up to 99 channels (typical 42) → dλ ~ 0.07Å for @ 42 TOF chan.	mu metal shielding, shielding factor 137 → echo phase stability

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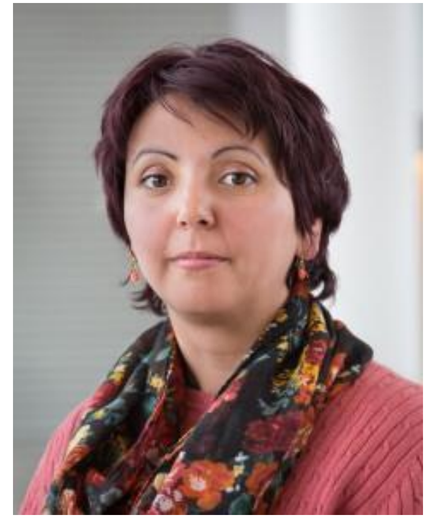
SNS-NSE Instrument Team



Piotr Adam Zolnierczuk (Instrument Scientist)

Mary Odom (Scientific Associate)

Laura-Roxana Stingaciu (Instrument Scientist)

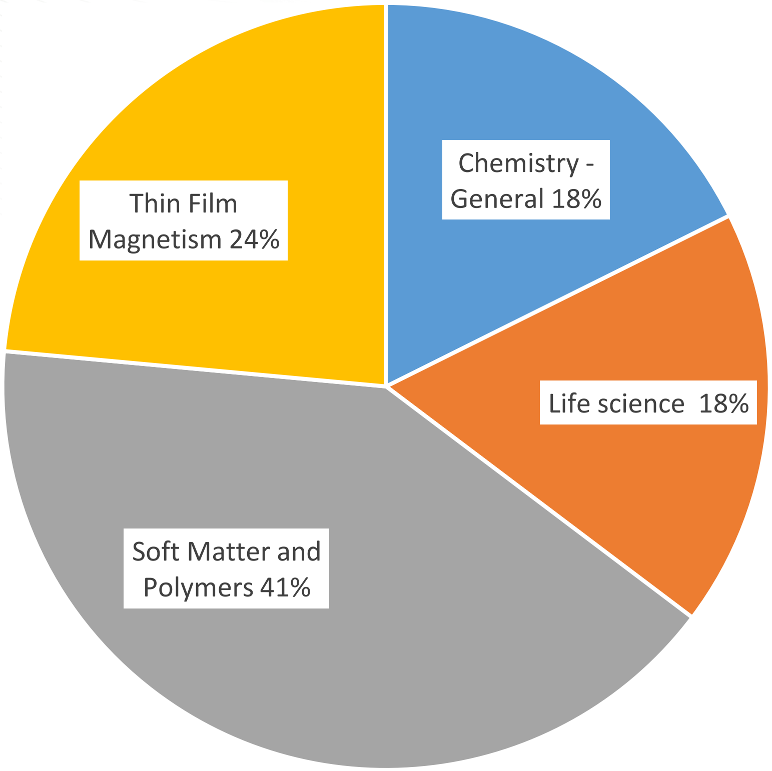
Over the past three years:

Wei-Ren Chen, Instrument Scientist

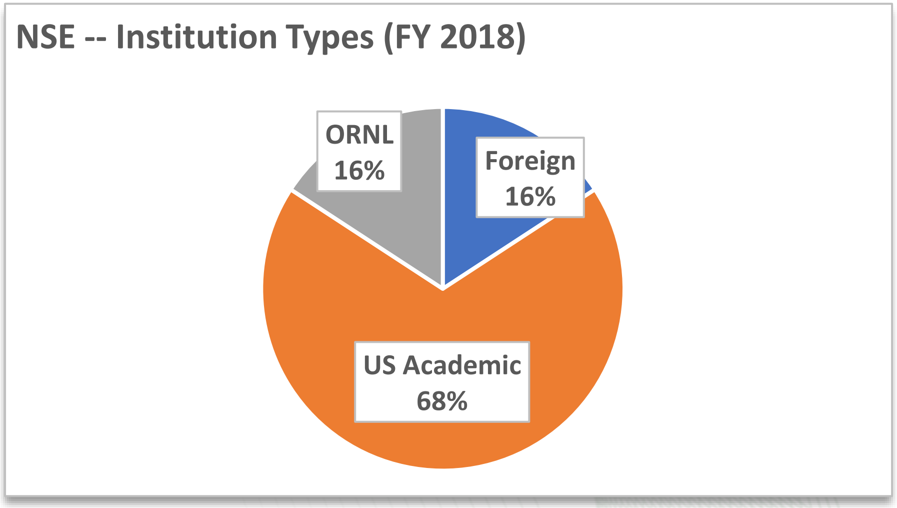
Malcolm Cochran, Scientific Associate

Scientific Mission and Impact

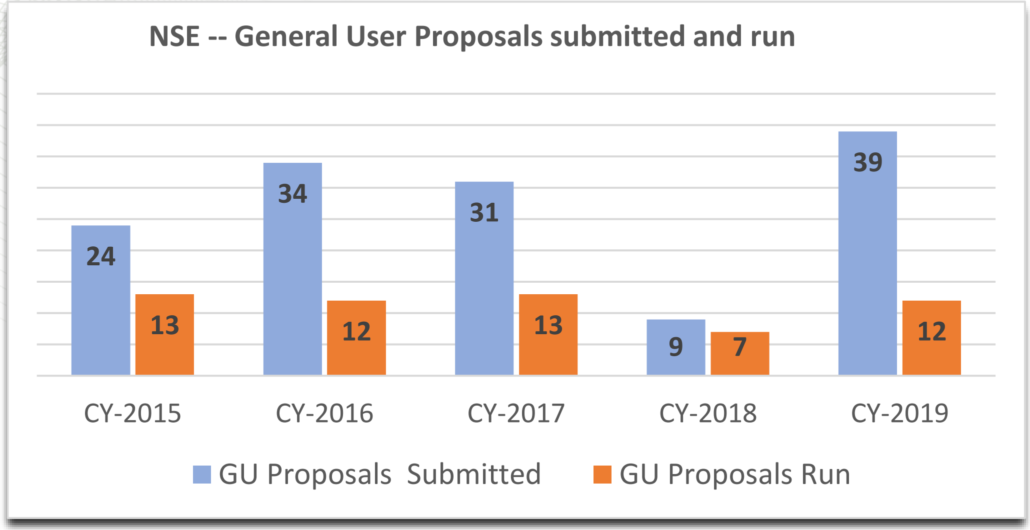
NSE Research Areas (2019)

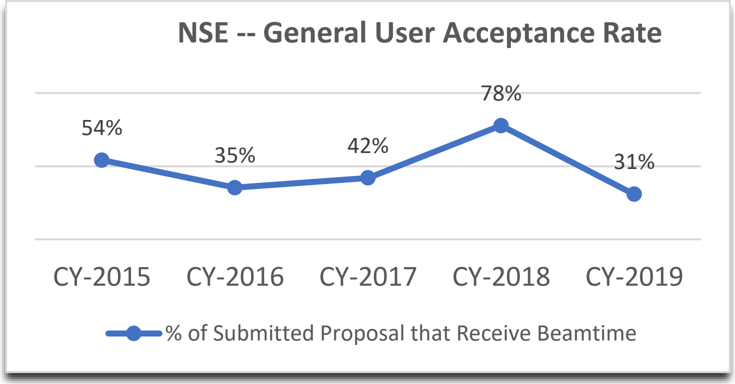


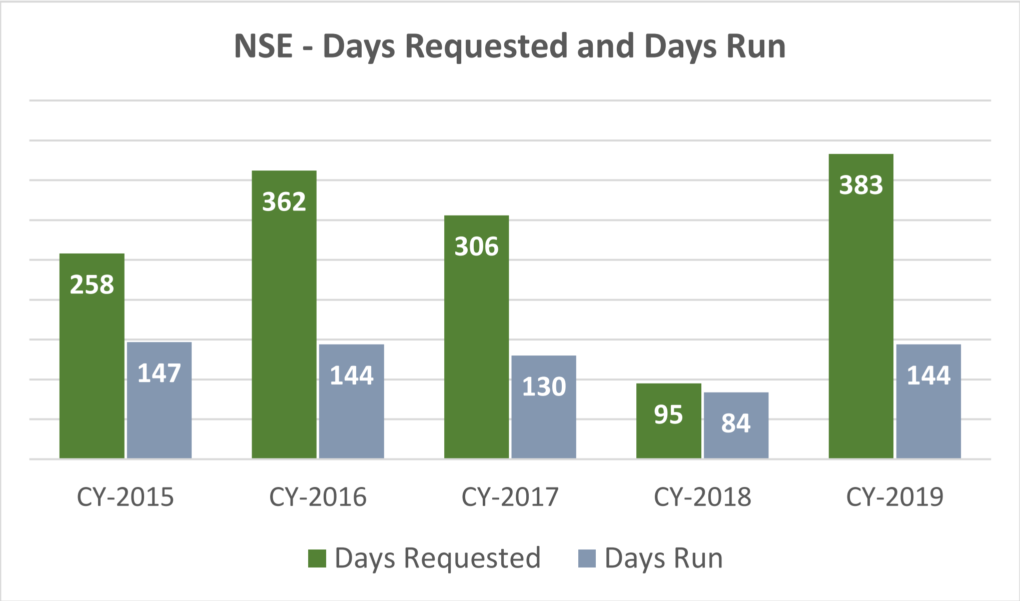
- The SNS-NSE instrument is used to answer scientific questions in a variety of fields like soft-matter research, biophysics, materials science, chemistry, complex fluids, and is particularly suitable to unravel slow dynamical processes and molecular motions at nanoscopic and mesoscopic scale.

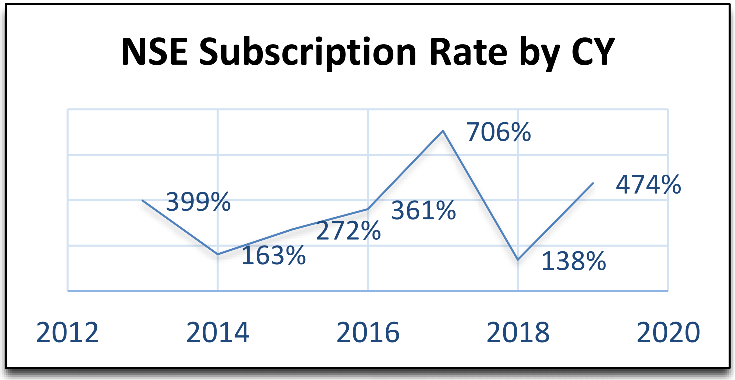


GU Program Quality and Beam Time Usage







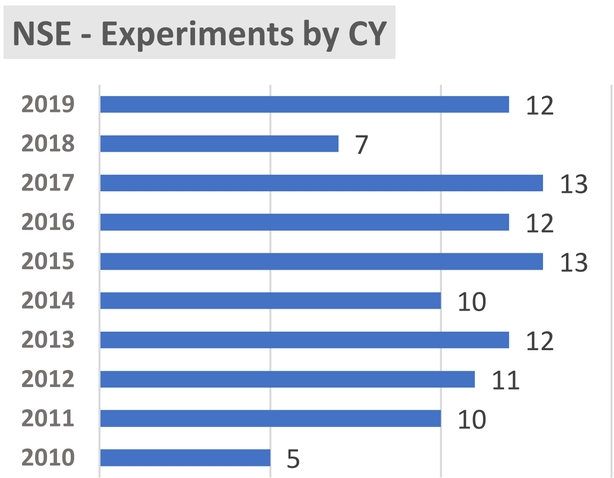


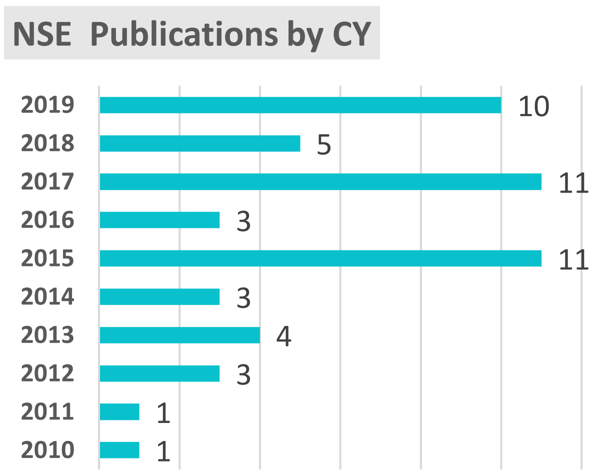
- Subscription Rate, 7-year average (nr. of requested days/nr. of available days): **359%**

SNS-NSE Beamline Productivity

- Total Publications: **56**
- Instrument H-Index: **12**
- Publication Impact: **12%** publications with a high impact factor (recent 3 years)
- Results from use of multiple instruments: **45%**
- Unique authors 2017-2019: **98**

Other NSE's	2017	2018	2019
ILL - IN15	7	11	7
CHRNS - NSE	10	13	18
FRMII - NSE	8	7	11





SNS-NSE Software *DrSpine*
= Data Reduction For Spin Echo Experiments

research papers

JAC Appl Cryst
JOURNAL OF APPLIED CRYSTALLOGRAPHY

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Efficient data extraction from neutron time-of-flight spin-echo raw data

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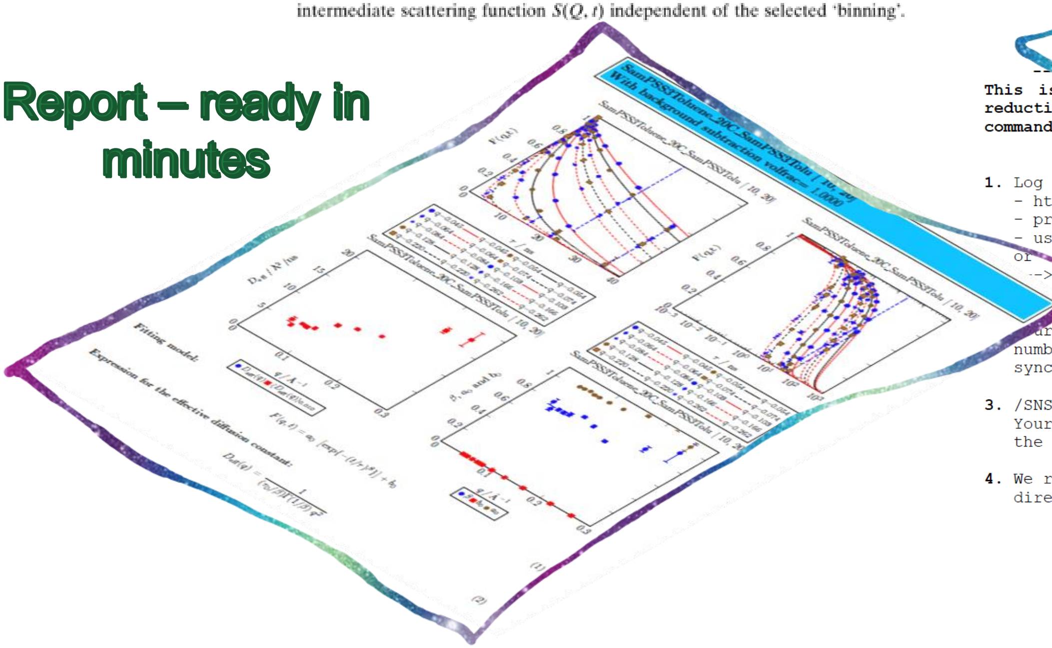
Supporting information: this article has supporting information at journals.iucr.org/j

Neutron spin-echo spectrometers with a position-sensitive detector and operating with extended time-of-flight-tagged wavelength frames are able to collect a comprehensive set of data covering a large range of wavevector and Fourier time space with only a few instrumental settings in a quasi-continuous way. Extracting all the information contained in the raw data and mapping them to a suitable physical space in the most efficient way is a challenge. This article reports algorithms employed in dedicated software, *DrSpine* (data reduction for spin echo), that achieves this goal and yields reliable representations of the intermediate scattering function $S(Q, t)$ independent of the selected 'binning'.

Macro Template
(or instructions how to generate a template macro

```
macro
clear all

c ==== set binning
bins pix nbins 8
bins tof custom 4 10 16 22 30 38
set bgr 1

c ==== read data
c ==== set paths for resolution, sample, buffer

datapath /SNS/NSE/IPTS-22xxx

! read resolution data
read s933x.echo s933x.echo as res     !8A
read s933x.echo            as res     !9A
read s933x.echo s933x.echo as res     !11A

! read sample1 data
read s934x.echo s934x.echo as sam tfac 0.9x    !8A
read s934x.echo            as sam tfac 0.9x    !9A
read s934x.echo s934x.echo as sam tfac 0.9x    !11A

! read buffer1 data
read s935x.echo s935x.echo as buf     !8A
read s935x.echo            as buf     !9A
read s935x.echo s935x.echo as buf     !11A

c === process data
match all
fit all
```

Report – ready in minutes



Quick Guide for drSpine   SNS-NSE   April 2019

This is a general guide to access the most common commands for drSpine data reduction software. For additional commands please see drSpine help by typing command ---> help into drSpine environment or ask the Instrument Scientist

1. Log in to Neutron Sciences Remote Analysis Cluster (on Windows)
   - https://analysis.sns.gov/
   - press Launch Session button
   - use ORNL user credential account details

   or
   --> ss -Y analysis.sns.gov (from a Linux terminal, with the same ORNL ntials)

ur raw data are uploaded and stored in /SNS/NSE/IPTS-XXXXX (your own IPTS number). Do not work in this directory, is overwrite whenever new data are sync

3. /SNS/NSE/shared/ is a shared users directory
   Your local contact will place here any data reduction; it will be named with the appropriate IPTS number; you can work here and modify as you like

4. We recommend best create a folder for your data reduction in your Home user directory and work there ....

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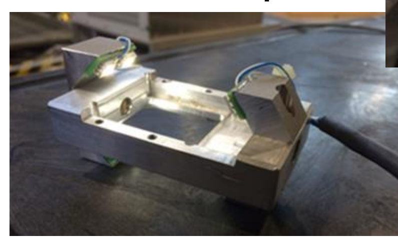
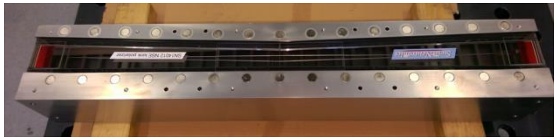
Sample Environment

- Temperature Forcing System
  - Fast sample change
  - < 0.1°C accuracy across the range
  - Sample container ramps from 0°C to 150°C within 8 minutes
- Janis Cryostat 3.5K – 650K
- Light Cell
  - Allows adaptation of photosensitive samples
  - Delivers 30 - 1700 μE
  - Operated remotely
- Tumbler
  - Stir samples during the collection of NSE spectra
  - Rotates from < 20 to > 800 rpm with temperature stability < 0.2°C
- Humidity chamber with non-reactive atmosphere



Ancillary Equipment and Upgrades



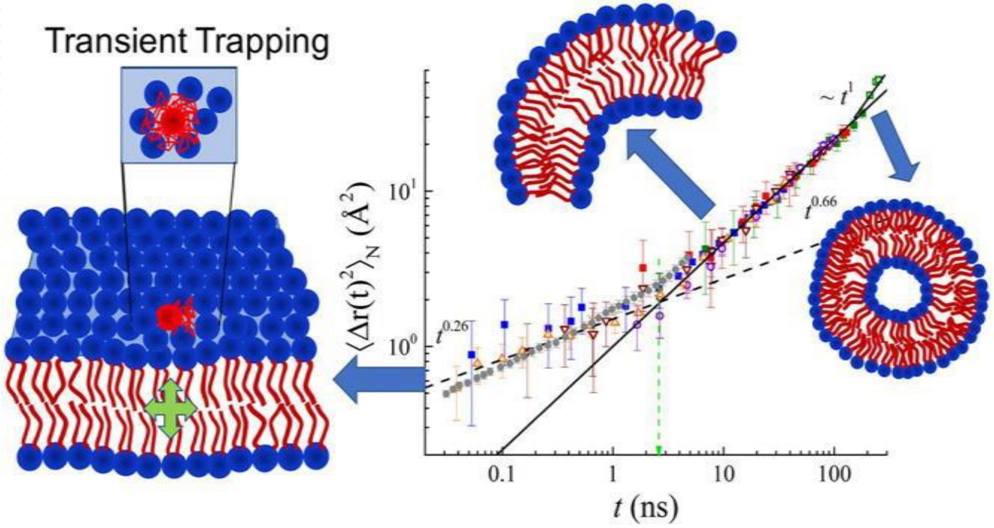
- Shorty mode of operation option
- New bender polarizer (f.r. 72.8%, fl.16.9%)
- Neutron camera improved software for real time positioning of the sample
- Upgrade of cryo-furnace heating elements and sample can for reaching temperatures below 5K
- New upgraded sample holder for Temperature Forcing System (TFS), for better insulation and improve beam transparency

- New heater arm for TFS
- Testing new CAENels power supply
- New mechanical holders to host grazing incidence cell
- New mechanical holders fabricated to manually adjust alignment of crystals into NSE spectrometer
- New stretching device for polymer samples in the beam
- Inventory of all equipment, parts, tools, and supplies for transition

Research Highlights

- Dynamics of Phospholipid Membranes beyond Thermal Undulations
- Osmolyte Interactions in Intrinsically Disordered Myelin Basic Protein
- Inner Dynamics of Crosslinked PNIPAM Microgels with High Crosslinker Content

Dynamics of Phospholipid Membranes beyond Thermal Undulations



The Proposed mechanism of transient trapping and mean square displacement ⟨Δr(t)^2 ⟩N as a function of Fourier time.

Research Details

The molecular dynamics of unilamellar liposomes was investigated and compared to MD simulations

Scientific Achievement

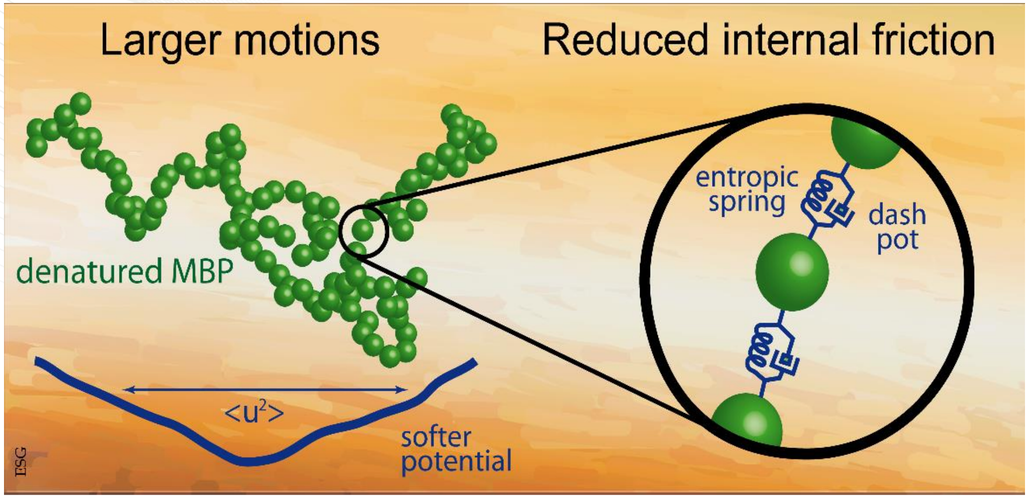
The reported mean squared displacement shows a $t^{0.26}$ dependence in the pico-to-nanosecond region, that points to another process beyond the well-established model of thermal membrane undulation of Zilman and Granek (ZG). Comparison to MD associates the observed low exponent with a non-Gaussian transient trapping of the lipids.

Significance and Impact

The study shows that friction at the interface between water and liposomes plays a minor role. The center of mass diffusion of liposomes and transient trapping of lipids define the range in which the ZG model can be applied.

Sudipta Gupta, Judith U. De Mel, Rasangi M. Perera, Piotr Zolnierczuk, Markus Bleuel, Antonio Faraone, and Gerald J. Schneider, J. Phys. Chem. Lett. 9, 2956 (2018)

Osmolyte Interactions in the Intrinsically Disordered Myelin Basic Protein



Energy landscape of intrinsically denatured Myelin Basic Protein exhibits a softened, shallow energy landscape (lower left) leading to the characteristic mechanical behavior of an entropic spring with large amplitude motions.

Scientific Achievement

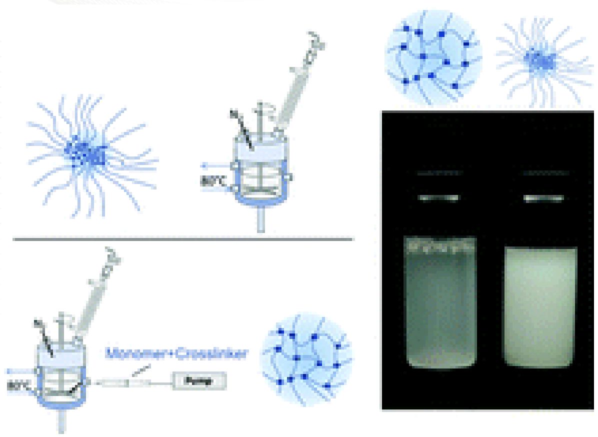
It was shown that the relaxation time and amplitude of internal motions in myelin basic protein (MBP) increase upon urea denaturation leading to synthetic polymer-like behavior of the unfolded protein.

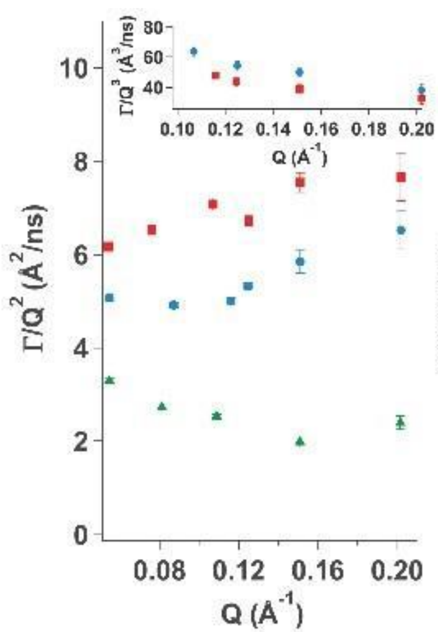
Significance and Impact

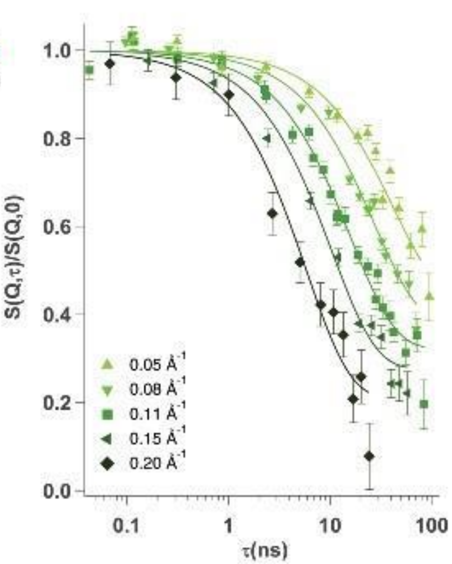
This work sheds light on the functionality of MBP in the myelin sheath membrane surrounding nerves, yielding information important for understanding demyelinating diseases.

L. R. Stingaciu, R. Biehl, D. Changwoo, D. Richter, A. M. Stadler, J. Phys. Chem. Lett. 2020, ***11****, 292−296 (2020) DOI: 10.1021/acs.jpclett.9b03001*

Inner Dynamics of Crosslinked PNIPAM Microgels with High Crosslinker Content







Scientific Achievement

Dynamic Light Scattering, atomic force microscopy and Small Angle Neutron Scattering were conducted and related to neutron spin echo spectroscopy data. A link between structural and dynamic features of the internal polymer network was made:

- A dominance of the cooperative cooperative density dynamics with a simple Q^2 dependence in dense core microgels
- A Zimm-type dynamics in microgels obtained by continuous monomer feeding approach

Judith Witte, Stefan Wellert,…et al., Soft Matter, 15, 1053 (2019), https://doi.org/10.1039/C8SM02141D

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Future Instrument Development Plans

- Power upgrade: new system manufactured by CAENels offer stability, resolution, and operational flexibility

✓ mid-scale proposal submitted

✓ purchased started for off-the-shelf units

- Install upgraded chopper 1 disc (carbon fiber)
- Analyzer upgrades
- Software improvement for data acquisition - EPICS
- MORE sample environments *--- based on users input*
  - Electric Field Cell
  - Pressure Cell
  - Rheometer
  - Furnace 1000 °C

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Overall Summary & Vision

- The NSE technique is in high demand and has the potential for increased throughput
- SNS-NSE is in high demand and constantly overbooked
- With the recent technical upgrades, new and improved data reduction software, and the development and integration of more accessible sample environments SNS-NSE instruments becoming more intuitive for expert and novice users alike

Our NSE Vision is a "***Neutron Spin Echo Center of Excellence @ ORNL"*** within the next 5 - 10 years, with two high resolution NSE spectrometers, with complementary characteristics separated by scientific applications.

THANK YOU